



Full wwPDB EM Validation Report ⓘ

Jul 19, 2026 – 04:36 pm BST

PDB ID : 9S1L / pdb_00009s1l
EMDB ID : EMD-54455
Title : Cryo-EM structure of Posidonia oceanica PSI-LHCI supercomplex
Authors : Capaldi, S.; Amelii, A.; Sanita, G.; Esposito, M.; Bassi, R.
Deposited on : 2025-07-18
Resolution : 2.83 Å(reported)
Based on initial model : 5ZJI

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

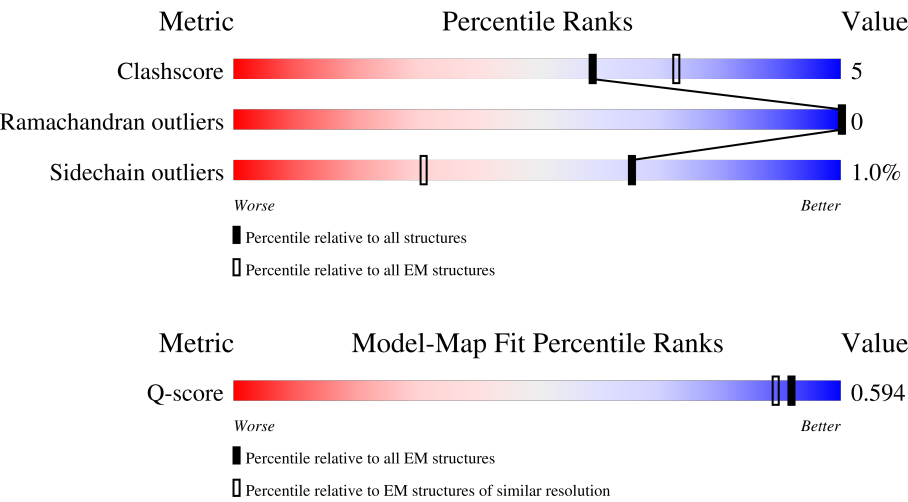
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



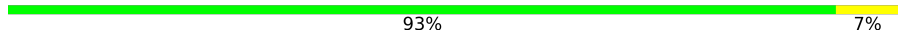
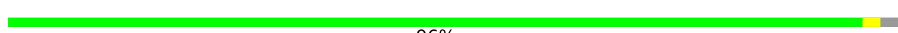
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11847 (2.33 - 3.33)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	200	89%8%
2	2	211	87%9%
3	3	232	20% 80%12%8%
4	4	200	90%8%

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Mol	Chain	Length	Quality of chain
5	A	750	
6	B	734	
7	C	81	
8	D	155	
9	E	93	
10	F	159	
11	G	100	
12	H	95	
13	I	36	
14	J	42	
15	K	84	
16	L	170	

2 Entry composition [i](#)

There are 27 unique types of molecules in this entry. The entry contains 35475 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Chlorophyll a-b binding protein 6, chloroplastic (Lhca1).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	194	Total	C	N	O	S	0	0
			1504	981	252	266	5		

- Molecule 2 is a protein called Photosystem I chlorophyll a/b-binding protein 2 (Lhca2).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	203	Total	C	N	O	S	0	0
			1579	1031	257	285	6		

- Molecule 3 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	213	Total	C	N	O	S	0	0
			1638	1074	263	295	6		

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4 (Lhca4).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	198	Total	C	N	O	S	0	0
			1557	1017	254	283	3		

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1 (PsaA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	724	Total	C	N	O	S	0	0
			5684	3726	968	972	18		

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 (PsaB).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	733	Total	C	N	O	S	0	0
			5858	3847	996	1002	13		

- Molecule 7 is a protein called Photosystem I iron-sulfur center (PsaC).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	80	Total	C	N	O	S	0	0
			614	380	106	117	11		

- Molecule 8 is a protein called Photosystem I reaction center subunit II-1 (PsaD).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	140	Total	C	N	O	S	0	0
			1103	708	190	201	4		

- Molecule 9 is a protein called Photosystem I reaction center subunit IV A (PsaE1).

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	63	Total	C	N	O	0	0
			519	333	92	94		

- Molecule 10 is a protein called Photosystem I reaction center subunit III (PsaF).

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	155	Total	C	N	O	S	0	0
			1224	794	209	217	4		

- Molecule 11 is a protein called Photosystem I reaction center subunit V (PsaG).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	98	Total	C	N	O	S	0	0
			768	500	128	139	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit VI-1 (PsaH1).

Mol	Chain	Residues	Atoms				AltConf	Trace
12	H	94	Total	C	N	O	0	0
			736	483	114	139		

- Molecule 13 is a protein called Photosystem I reaction center subunit VIII (PsaI).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	32	Total	C	N	O	S	0	0
			246	167	39	39	1		

- Molecule 14 is a protein called Photosystem I reaction center subunit IX (PsaJ).

Mol	Chain	Residues	Atoms				AltConf	Trace
14	J	40	Total	C	N	O	0	0
			319	216	49	54		

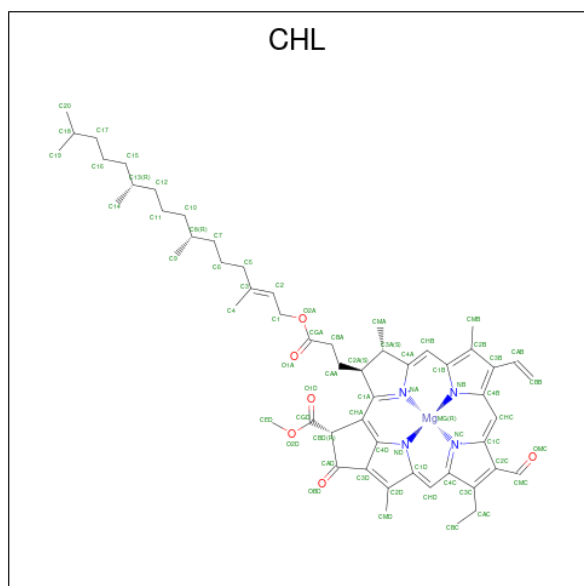
- Molecule 15 is a protein called Photosystem I reaction center subunit psaK (PsaK).

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	55	Total	C	N	O	S	0	0
			386	251	62	69	4		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI (PsaL).

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	152	Total	C	N	O	S	0	0
			1141	755	179	204	3		

- Molecule 17 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



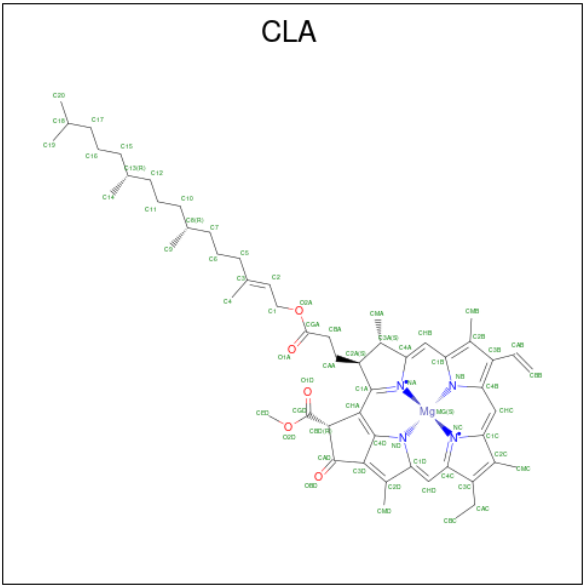
Mol	Chain	Residues	Atoms					AltConf
17	1	1	Total	C	Mg	N	O	0
			55	44	1	4	6	
17	1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	2	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
17	3	1	Total	C	Mg	N	O	0
			47	36	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			56	45	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
17	4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	

- Molecule 18 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	3	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
18	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	4	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 42	C 34	Mg 1	N 4	O 3	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	A	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
18	B	1	Total 43	C 35	Mg 1	N 4	O 3	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 59	C 49	Mg 1	N 4	O 5	0
18	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
18	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
18	B	1	Total 50	C 40	Mg 1	N 4	O 5	0

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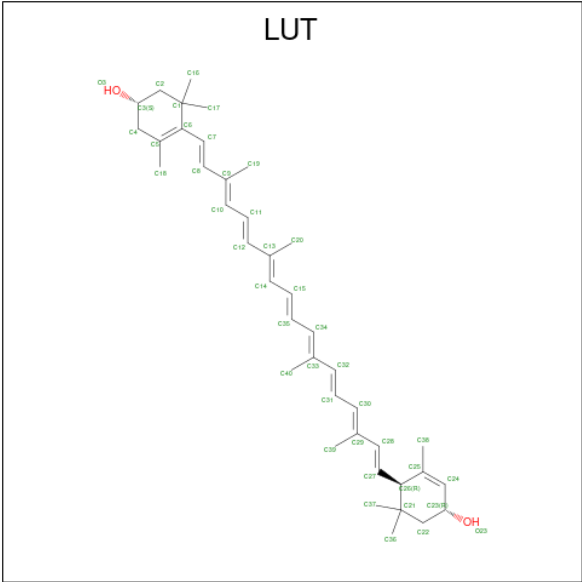
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			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
18	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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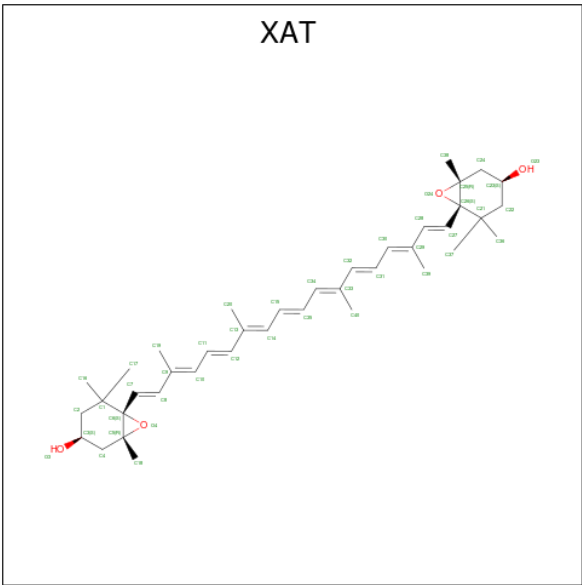
Mol	Chain	Residues	Atoms					AltConf
18	F	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
18	F	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	F	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	G	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	H	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
18	J	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
18	K	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
18	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
18	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 19 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



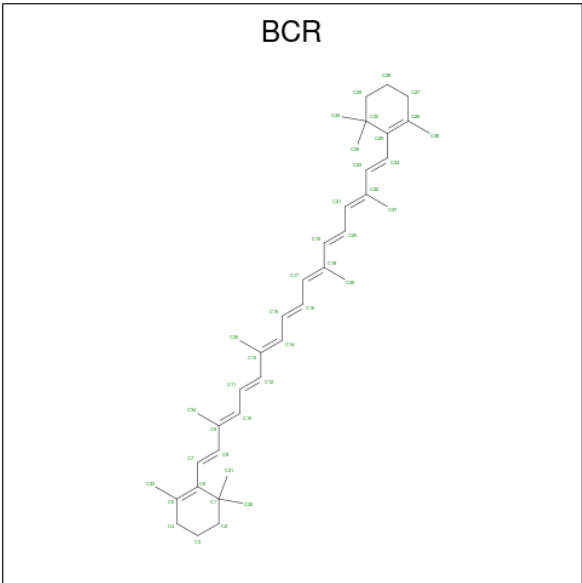
Mol	Chain	Residues	Atoms			AltConf
19	1	1	Total	C	O	0
			42	40	2	
19	1	1	Total	C	O	0
			42	40	2	
19	2	1	Total	C	O	0
			42	40	2	
19	3	1	Total	C	O	0
			42	40	2	
19	4	1	Total	C	O	0
			42	40	2	

- Molecule 20 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
20	1	1	Total	C	O	0
			44	40	4	
20	2	1	Total	C	O	0
			44	40	4	
20	3	1	Total	C	O	0
			44	40	4	
20	4	1	Total	C	O	0
			44	40	4	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆) (labeled as "Ligand of Interest" by depositor).



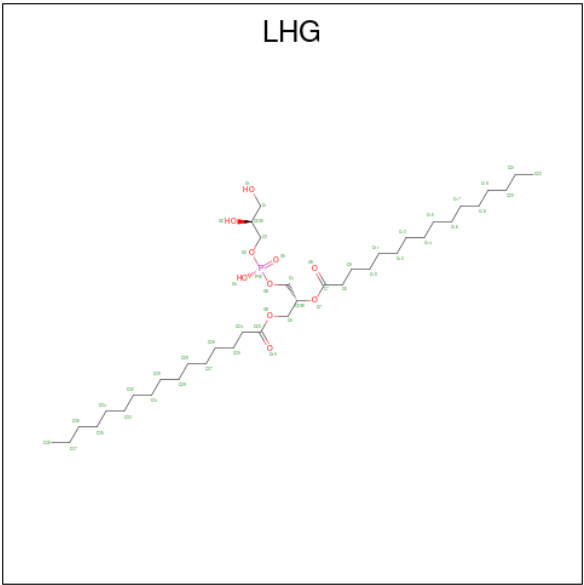
Mol	Chain	Residues	Atoms	AltConf
21	1	1	Total C 40 40	0
21	2	1	Total C 40 40	0
21	3	1	Total C 40 40	0
21	4	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	F	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	J	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
21	K	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



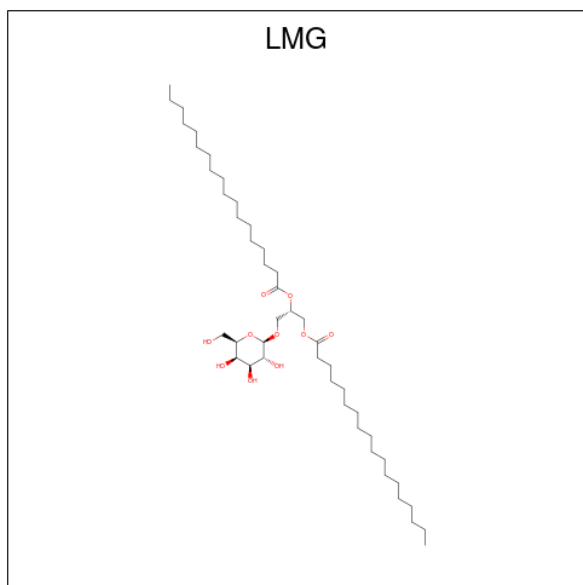
Mol	Chain	Residues	Atoms	AltConf
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 49 38 10 1	0
22	1	1	Total C O P 38 27 10 1	0
22	2	1	Total C O P 37 26 10 1	0
22	A	1	Total C O P 49 38 10 1	0

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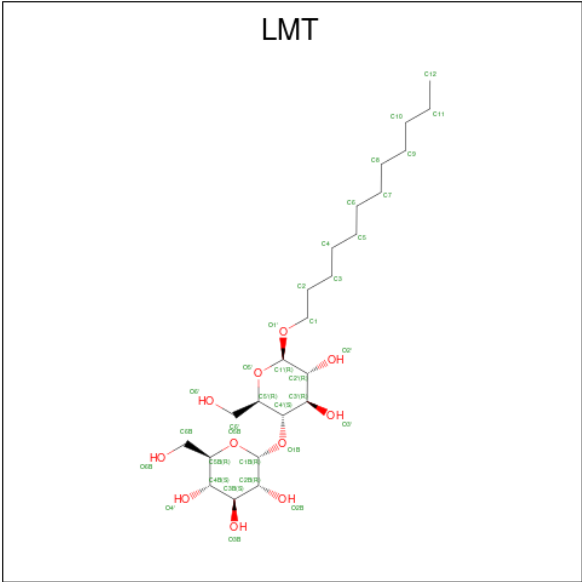
Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	O	P	0
			30	19	10	1	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



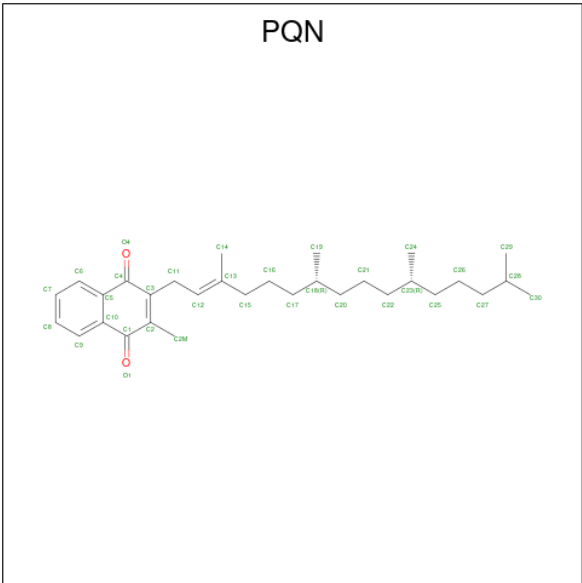
Mol	Chain	Residues	Atoms			AltConf
23	1	1	Total	C	O	0
			53	43	10	
23	1	1	Total	C	O	0
			50	40	10	
23	4	1	Total	C	O	0
			36	26	10	
23	4	1	Total	C	O	0
			49	39	10	
23	B	1	Total	C	O	0
			52	42	10	
23	F	1	Total	C	O	0
			47	37	10	
23	F	1	Total	C	O	0
			30	20	10	

- Molecule 24 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



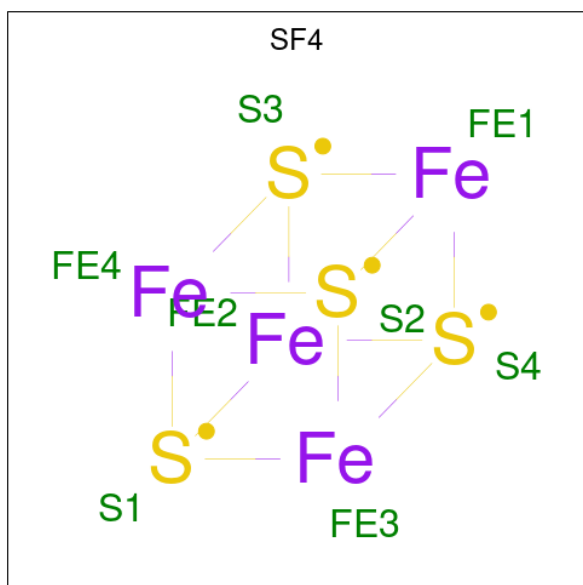
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			35	24	11	
24	G	1	Total	C	O	0
			35	24	11	

- Molecule 25 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Lig- and of Interest" by depositor).



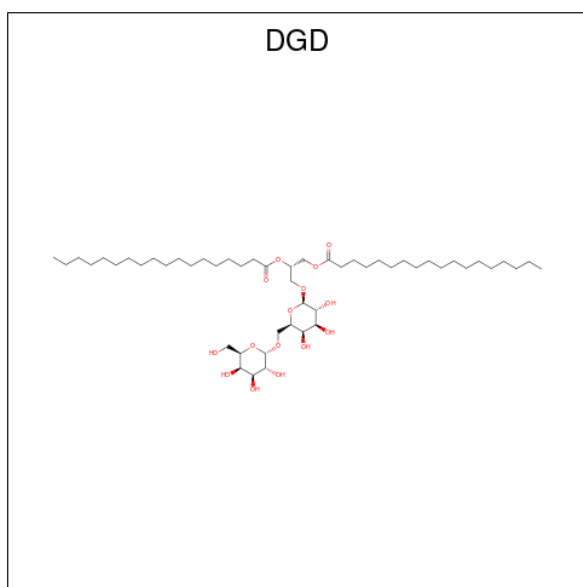
Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	O	0
			33	31	2	
25	B	1	Total	C	O	0
			33	31	2	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
26	A	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	
26	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 27 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $\text{C}_{51}\text{H}_{96}\text{O}_{15}$) (labeled as "Ligand of Interest" by depositor).



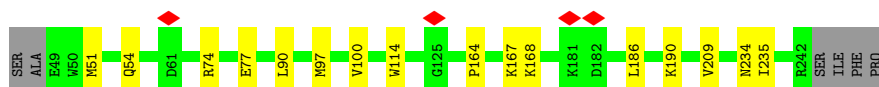
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
27	B	1	61	46	15	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Chlorophyll a-b binding protein 6, chloroplastic (Lhca1)

Chain 1: 



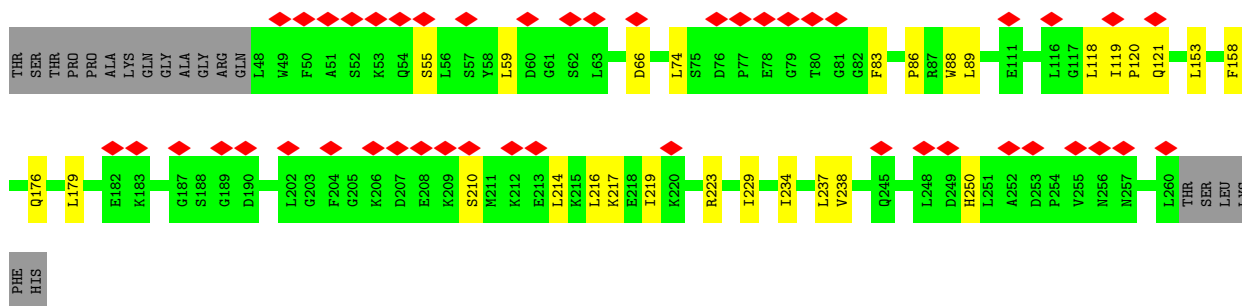
- Molecule 2: Photosystem I chlorophyll a/b-binding protein 2 (Lhca2)

Chain 2: 



- Molecule 3: Photosystem I chlorophyll a/b-binding protein 3-1 (Lhca3)

Chain 3: 



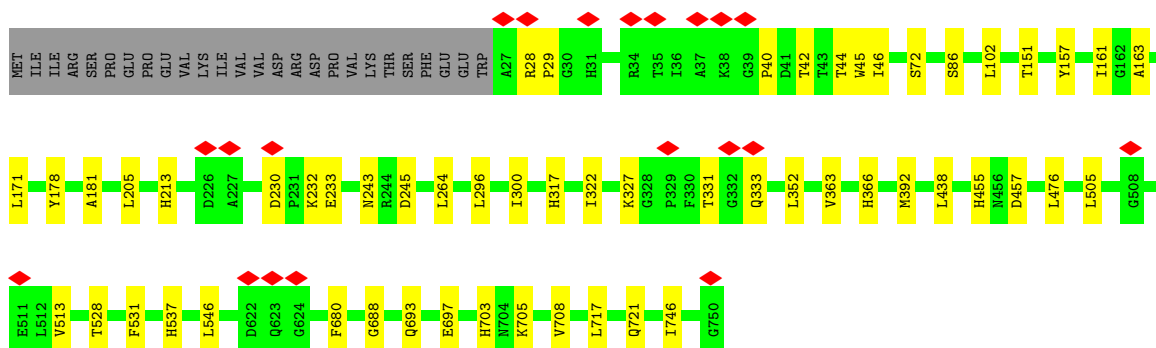
- Molecule 4: Chlorophyll a-b binding protein 4 (Lhca4)

Chain 4: 



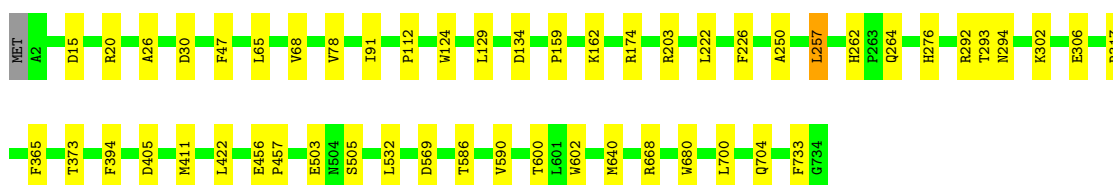
- Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1 (PsaA)

Chain A:  89% 7%



- Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2 (PsaB)

Chain B:  93% 7%



- Molecule 7: Photosystem I iron-sulfur center (PsaC)

Chain C:  85% 14%



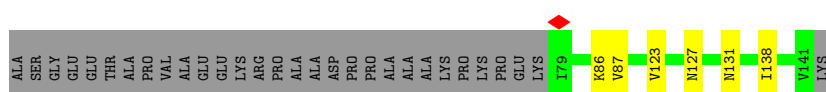
- Molecule 8: Photosystem I reaction center subunit II-1 (PsaD)

Chain D:  81% 9% 10%



- Molecule 9: Photosystem I reaction center subunit IV A (PsaE1)

Chain E:  61% 6% 32%



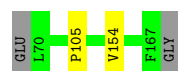
- Molecule 10: Photosystem I reaction center subunit III (PsaF)

Chain F:  9% 88% 9%



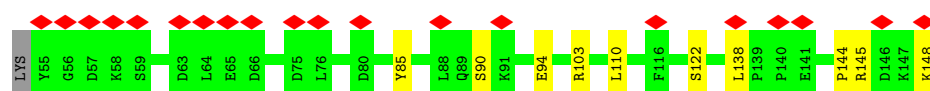
- Molecule 11: Photosystem I reaction center subunit V (PsaG)

Chain G: 96% ..



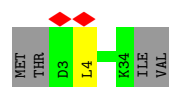
- Molecule 12: Photosystem I reaction center subunit VI-1 (PsaH1)

Chain H: 21% 88% 11% .



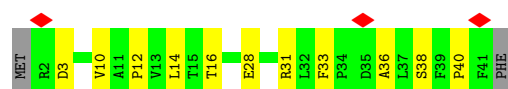
- Molecule 13: Photosystem I reaction center subunit VIII (PsaI)

Chain I: 6% 86% 11% .



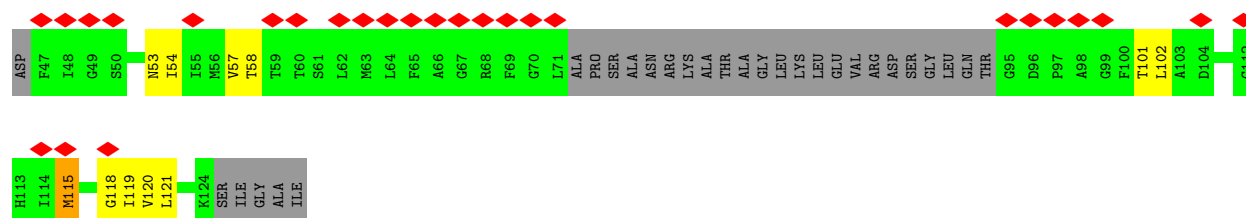
- Molecule 14: Photosystem I reaction center subunit IX (PsaJ)

Chain J: 7% 69% 26% 5%



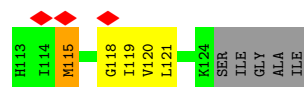
- Molecule 15: Photosystem I reaction center subunit psaK (PsaK)

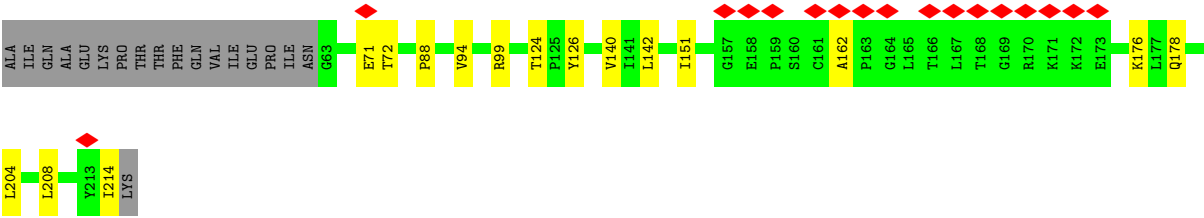
Chain K: 32% 52% 12% 35%



- Molecule 16: Photosystem I reaction center subunit XI (PsaL)

Chain L: 10% 80% 9% 11%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	120603	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	750	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	40.986	Depositor
Minimum map value	-19.686	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.986	Depositor
Recommended contour level	4.3	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92, 0.92, 0.92	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, PQN, XAT, CLA, DGD, SF4, LUT, CHL, LHG, BCR, LMG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.15	0/1553	0.29	0/2119
2	2	0.15	0/1634	0.29	0/2236
3	3	0.14	0/1690	0.31	0/2292
4	4	0.15	0/1606	0.30	0/2191
5	A	0.17	0/5878	0.32	0/8020
6	B	0.18	0/6070	0.33	0/8291
7	C	0.17	0/626	0.40	0/849
8	D	0.14	0/1131	0.38	0/1530
9	E	0.14	0/531	0.29	0/721
10	F	0.17	0/1253	0.36	0/1691
11	G	0.12	0/788	0.27	0/1069
12	H	0.11	0/759	0.28	0/1030
13	I	0.14	0/252	0.30	0/343
14	J	0.15	0/328	0.34	0/448
15	K	0.11	0/390	0.25	0/525
16	L	0.11	0/1176	0.27	0/1608
All	All	0.16	0/25665	0.32	0/34963

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1504	0	1491	12	0
2	2	1579	0	1524	12	0
3	3	1638	0	1602	20	0
4	4	1557	0	1519	12	0
5	A	5684	0	5539	39	0
6	B	5858	0	5635	32	0
7	C	614	0	593	8	0
8	D	1103	0	1114	10	0
9	E	519	0	512	5	0
10	F	1224	0	1257	13	0
11	G	768	0	748	2	0
12	H	736	0	723	8	0
13	I	246	0	265	1	0
14	J	319	0	330	11	0
15	K	386	0	404	8	0
16	L	1141	0	1143	11	0
17	1	96	0	68	1	0
17	2	226	0	150	5	0
17	3	47	0	31	1	0
17	4	194	0	138	5	0
18	1	628	0	553	8	0
18	2	458	0	400	5	0
18	3	601	0	463	7	0
18	4	548	0	451	3	0
18	A	2510	0	2449	37	0
18	B	2282	0	2215	36	0
18	F	140	0	113	1	0
18	G	132	0	97	1	0
18	H	51	0	41	3	0
18	J	42	0	31	1	0
18	K	128	0	91	4	0
18	L	150	0	125	3	0
19	1	84	0	112	8	0
19	2	42	0	56	1	0
19	3	42	0	56	4	0
19	4	42	0	56	5	0
20	1	44	0	56	0	0
20	2	44	0	56	1	0
20	3	44	0	56	3	0
20	4	44	0	56	0	0
21	1	40	0	56	1	0
21	2	40	0	56	5	0
21	3	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	4	40	0	56	0	0
21	A	240	0	336	15	0
21	B	240	0	336	9	0
21	F	80	0	112	2	0
21	G	40	0	56	1	0
21	I	40	0	56	0	0
21	J	80	0	112	8	0
21	K	80	0	112	3	0
21	L	160	0	224	7	0
22	1	136	0	194	4	0
22	2	37	0	44	3	0
22	A	79	0	104	3	0
23	1	103	0	149	2	0
23	4	85	0	113	0	0
23	B	52	0	77	2	0
23	F	77	0	97	2	0
24	4	35	0	46	0	0
24	A	70	0	92	1	0
24	G	35	0	46	0	0
25	A	33	0	46	0	0
25	B	33	0	46	2	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	B	61	0	83	2	0
All	All	35475	0	35024	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:L:124:THR:HG22	16:L:126:TYR:H	1.43	0.82
6:B:262:HIS:HD2	6:B:264:GLN:H	1.30	0.81
14:J:10:VAL:HG12	14:J:12:PRO:HD2	1.67	0.76
19:3:614:LUT:H171	19:3:614:LUT:H8	1.68	0.75
6:B:411:MET:HE2	21:B:845:BCR:H292	1.68	0.74
8:D:149:ARG:HD2	8:D:157:GLN:HE21	1.53	0.74
5:A:327:LYS:HD3	5:A:333:GLN:HG2	1.70	0.73
4:4:108:VAL:HG11	19:4:616:LUT:H12	1.71	0.72
6:B:159:PRO:HA	6:B:162:LYS:HE2	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:2:617:LHG:HC81	21:3:601:BCR:HC42	1.73	0.69
7:C:66:ARG:HD3	8:D:184:ILE:HD11	1.73	0.69
12:H:103:ARG:HD3	16:L:151:ILE:HG12	1.72	0.69
8:D:160:HIS:HB3	8:D:161:PRO:HD3	1.76	0.67
5:A:537:HIS:HB3	18:A:837:CLA:HBB1	1.77	0.66
10:F:107:LEU:HB2	10:F:120:ILE:HG21	1.78	0.66
4:4:122:ILE:HG13	4:4:123:ILE:HG23	1.78	0.65
17:4:605:CHL:HBB2	17:4:606:CHL:HBB1	1.77	0.65
1:1:186:LEU:HG	1:1:190:LYS:HE2	1.78	0.64
5:A:327:LYS:H	18:A:854:CLA:HBC3	1.63	0.64
4:4:244:HIS:HA	4:4:249:GLN:HE22	1.63	0.64
6:B:257:LEU:HD13	18:B:816:CLA:HMB3	1.79	0.64
18:3:602:CLA:H62	20:3:615:XAT:H28	1.80	0.62
16:L:162:ALA:HB2	16:L:178:GLN:HG3	1.80	0.62
12:H:145:ARG:HH21	12:H:148:LYS:HG2	1.65	0.62
3:3:229:ILE:HG21	20:3:615:XAT:H12	1.80	0.61
18:A:808:CLA:H12	18:A:810:CLA:H2	1.84	0.60
15:K:53:ASN:O	15:K:57:VAL:HG23	2.01	0.60
6:B:30:ASP:HB3	18:B:828:CLA:HAA2	1.83	0.60
18:B:811:CLA:HAC2	18:B:812:CLA:HAB	1.84	0.59
18:B:821:CLA:HBA1	18:B:821:CLA:HBD	1.85	0.59
18:B:807:CLA:H43	18:B:826:CLA:H11	1.83	0.58
6:B:276:HIS:HB2	18:B:816:CLA:C1B	2.33	0.58
14:J:38:SER:O	21:J:101:BCR:H10C	2.03	0.58
5:A:680:PHE:HA	18:A:802:CLA:HAB	1.85	0.58
21:K:204:BCR:H382	21:K:204:BCR:H23C	1.85	0.58
3:3:210:SER:O	3:3:214:LEU:HD12	2.03	0.58
3:3:74:LEU:HD21	18:A:812:CLA:H42	1.85	0.58
5:A:42:THR:HG22	5:A:44:THR:H	1.68	0.58
7:C:15:THR:HA	7:C:28:MET:HE3	1.86	0.58
21:A:850:BCR:H352	21:A:850:BCR:H10C	1.85	0.58
6:B:317:ARG:HG3	6:B:405:ASP:HB3	1.86	0.58
1:1:100:VAL:HG11	19:1:615:LUT:H12	1.86	0.57
10:F:201:VAL:HG21	23:F:307:LMG:H112	1.87	0.57
10:F:115:ALA:HA	10:F:118:LEU:HD12	1.86	0.56
12:H:122:SER:HA	21:L:301:BCR:H322	1.88	0.56
6:B:292:ARG:HD3	11:G:105:PRO:HD3	1.87	0.56
5:A:40:PRO:O	10:F:193:THR:HG21	2.06	0.56
17:2:601:CHL:HHC	17:2:601:CHL:HBB1	1.88	0.55
1:1:209:VAL:HG13	19:1:619:LUT:H162	1.88	0.55
10:F:120:ILE:O	10:F:124:MET:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B:809:CLA:HBA2	18:B:809:CLA:HBD	1.87	0.55
5:A:243:ASN:ND2	5:A:245:ASP:H	2.04	0.55
5:A:708:VAL:HG12	10:F:180:ARG:HG3	1.89	0.55
18:A:843:CLA:H2	21:A:849:BCR:H362	1.87	0.55
2:2:207:ILE:O	2:2:211:ARG:HG3	2.06	0.54
18:A:828:CLA:H171	21:J:103:BCR:H17C	1.90	0.54
6:B:293:THR:HG22	6:B:294:ASN:H	1.72	0.54
23:1:623:LMG:H121	11:G:154:VAL:HG22	1.90	0.54
18:B:825:CLA:H143	21:B:846:BCR:H17C	1.89	0.54
17:2:606:CHL:HHC	17:2:606:CHL:HBB1	1.90	0.54
5:A:230:ASP:HB3	5:A:233:GLU:HG2	1.89	0.54
12:H:90:SER:O	12:H:94:GLU:HG3	2.09	0.53
6:B:203:ARG:HG3	6:B:250:ALA:HB1	1.90	0.53
19:1:619:LUT:C8	19:1:619:LUT:H181	2.39	0.53
6:B:68:VAL:HG11	6:B:124:TRP:HZ3	1.74	0.53
5:A:72:SER:OG	5:A:178:TYR:HB2	2.09	0.53
6:B:302:LYS:O	6:B:306:GLU:HG2	2.08	0.53
18:B:839:CLA:HBC3	21:B:847:BCR:H21C	1.91	0.53
1:1:51:MET:HE3	1:1:54:GLN:HG3	1.92	0.52
1:1:234:ASN:HB2	18:1:613:CLA:HED1	1.92	0.52
5:A:102:LEU:HD11	5:A:151:THR:HA	1.91	0.52
3:3:216:LEU:O	3:3:219:ILE:HG13	2.10	0.52
3:3:234:ILE:HG21	18:3:611:CLA:HAC2	1.92	0.52
17:3:616:CHL:HHC	17:3:616:CHL:HBB1	1.92	0.52
18:B:829:CLA:HBB1	18:B:840:CLA:H13	1.92	0.51
7:C:61:ASP:HB3	9:E:131:ASN:ND2	2.26	0.51
14:J:40:PRO:HG2	21:J:101:BCR:H321	1.92	0.51
18:H:201:CLA:H2A	18:H:201:CLA:HED2	1.92	0.51
18:A:809:CLA:HAB	21:J:103:BCR:H352	1.93	0.51
19:1:619:LUT:H181	19:1:619:LUT:H8	1.93	0.51
3:3:250:HIS:CD2	18:3:611:CLA:HAA2	2.46	0.51
2:2:180:LYS:NZ	2:2:180:LYS:HB3	2.26	0.50
5:A:363:VAL:HG11	18:A:819:CLA:H191	1.94	0.50
12:H:85:TYR:HE2	16:L:94:VAL:HG11	1.77	0.50
8:D:150:VAL:HG22	8:D:156:VAL:HG12	1.92	0.50
14:J:38:SER:O	14:J:40:PRO:HD3	2.12	0.50
2:2:206:LYS:O	2:2:209:GLU:HG3	2.11	0.50
5:A:531:PHE:CZ	21:A:850:BCR:H322	2.47	0.50
18:A:854:CLA:HMA1	22:A:855:LHG:HC82	1.93	0.50
18:A:810:CLA:HAA1	18:A:810:CLA:HBD	1.94	0.49
21:L:305:BCR:H392	21:L:305:BCR:H23C	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:A:821:CLA:HBC3	18:A:827:CLA:H193	1.92	0.49
7:C:61:ASP:HB3	9:E:131:ASN:HD21	1.77	0.49
1:1:90:LEU:HD12	1:1:168:LYS:HG2	1.95	0.49
22:1:618:LHG:H211	22:1:618:LHG:H382	1.94	0.49
4:4:83:LEU:HD13	18:4:602:CLA:H42	1.94	0.49
6:B:129:LEU:HD23	6:B:134:ASP:HB3	1.93	0.49
2:2:135:GLU:OE2	2:2:135:GLU:HA	2.13	0.49
5:A:86:SER:HB2	5:A:163:ALA:HB3	1.95	0.49
3:3:234:ILE:O	3:3:238:VAL:HG22	2.12	0.49
18:A:803:CLA:H203	21:B:847:BCR:H321	1.95	0.49
18:A:817:CLA:H61	18:A:817:CLA:H41	1.57	0.49
2:2:229:TRP:O	2:2:233:ILE:HG22	2.12	0.49
6:B:373:THR:HG22	18:B:826:CLA:HAB	1.94	0.49
18:B:809:CLA:H62	21:L:301:BCR:HC7	1.95	0.48
19:2:615:LUT:C8	19:2:615:LUT:H181	2.43	0.48
18:B:821:CLA:HBB1	18:B:840:CLA:HED2	1.95	0.48
7:C:62:PHE:HD2	8:D:184:ILE:HG21	1.78	0.48
18:2:612:CLA:H92	18:2:612:CLA:H61	1.71	0.48
17:2:614:CHL:HHC	17:2:614:CHL:HBB1	1.95	0.48
5:A:264:LEU:HD13	15:K:120:VAL:HG11	1.95	0.48
22:A:855:LHG:H252	22:A:855:LHG:H101	1.94	0.48
2:2:209:GLU:OE1	2:2:213:LYS:HE2	2.14	0.47
5:A:205:LEU:HB3	21:A:846:BCR:H19C	1.96	0.47
18:A:841:CLA:H41	18:A:841:CLA:H61	1.61	0.47
2:2:189:PRO:HB3	17:2:607:CHL:HBC2	1.96	0.47
18:A:807:CLA:H112	18:A:807:CLA:H151	1.56	0.47
18:B:812:CLA:HBA1	18:B:812:CLA:H3A	1.48	0.47
18:B:817:CLA:H41	18:B:817:CLA:H62	1.63	0.47
19:1:615:LUT:C8	19:1:615:LUT:H181	2.45	0.47
15:K:54:ILE:O	15:K:58:THR:HG22	2.15	0.47
10:F:137:GLN:OE1	14:J:40:PRO:HG3	2.15	0.47
8:D:149:ARG:HD2	8:D:157:GLN:NE2	2.27	0.47
6:B:174:ARG:HB2	18:B:812:CLA:HBC2	1.96	0.46
7:C:55:GLU:HB3	7:C:63:LEU:HD13	1.96	0.46
23:F:306:LMG:H112	23:F:306:LMG:HC8	1.67	0.46
16:L:71:GLU:CD	16:L:71:GLU:H	2.23	0.46
8:D:147:PHE:CZ	8:D:160:HIS:HB2	2.50	0.46
18:A:817:CLA:H51	15:K:121:LEU:HD13	1.96	0.46
6:B:680:TRP:HD1	8:D:84:LEU:HD11	1.80	0.46
3:3:214:LEU:HA	3:3:217:LYS:HE2	1.98	0.46
18:B:826:CLA:H3A	18:B:826:CLA:HBA2	1.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:J:31:ARG:HB3	18:J:102:CLA:HED3	1.98	0.46
1:1:74:ARG:HA	1:1:74:ARG:HD3	1.64	0.46
4:4:83:LEU:HD21	10:F:213:ILE:HD13	1.98	0.46
21:A:849:BCR:H24C	21:A:849:BCR:H371	1.80	0.46
2:2:59:LEU:H	3:3:176:GLN:HE22	1.64	0.46
18:A:825:CLA:H193	18:A:825:CLA:H162	1.81	0.46
22:1:622:LHG:H311	18:B:840:CLA:H93	1.98	0.46
4:4:91:LYS:O	4:4:95:GLN:HG2	2.15	0.46
19:4:616:LUT:C8	19:4:616:LUT:H181	2.46	0.46
5:A:45:TRP:CE3	5:A:46:ILE:HG13	2.51	0.46
18:A:834:CLA:HBC2	18:B:809:CLA:HBC1	1.98	0.46
5:A:317:HIS:HB3	5:A:322:ILE:HD11	1.98	0.45
17:2:607:CHL:HMB2	21:2:618:BCR:H402	1.97	0.45
18:A:804:CLA:H62	18:A:804:CLA:H41	1.59	0.45
18:A:832:CLA:H8	21:L:306:BCR:H271	1.97	0.45
6:B:222:LEU:HD23	6:B:222:LEU:HA	1.82	0.45
18:3:611:CLA:C1B	19:3:614:LUT:H183	2.46	0.45
5:A:157:TYR:O	5:A:161:ILE:HG12	2.16	0.45
15:K:118:GLY:HA3	18:K:202:CLA:HBC2	1.97	0.45
23:1:620:LMG:H262	18:4:614:CLA:H2	1.98	0.45
5:A:746:ILE:HD12	5:A:746:ILE:HA	1.83	0.45
18:A:842:CLA:H193	18:A:842:CLA:H161	1.84	0.45
6:B:503:GLU:HG3	6:B:505:SER:H	1.80	0.45
9:E:123:VAL:HB	9:E:127:ASN:HA	1.98	0.45
5:A:476:LEU:HB2	5:A:528:THR:HG23	1.98	0.45
8:D:102:GLU:HA	8:D:115:MET:O	2.17	0.45
18:L:302:CLA:H3A	18:L:302:CLA:HBA2	1.66	0.45
2:2:150:LEU:HD23	2:2:150:LEU:HA	1.84	0.45
3:3:88:TRP:HE1	18:3:603:CLA:HED1	1.81	0.45
18:K:203:CLA:HBA1	18:K:203:CLA:H3A	1.49	0.45
17:4:607:CHL:H3A	17:4:607:CHL:HBA2	1.48	0.45
18:A:807:CLA:H2	18:A:807:CLA:HED2	1.98	0.45
21:A:847:BCR:H20C	21:A:847:BCR:H361	1.86	0.45
12:H:110:LEU:HD22	16:L:140:VAL:HG13	1.99	0.45
14:J:28:GLU:HA	14:J:28:GLU:OE2	2.17	0.45
17:1:606:CHL:HHC	17:1:606:CHL:HBB1	1.99	0.45
16:L:88:PRO:O	16:L:99:ARG:HD2	2.17	0.45
10:F:94:LYS:O	10:F:98:GLN:HG2	2.16	0.44
10:F:161:PHE:CE1	21:J:101:BCR:H372	2.52	0.44
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.99	0.44
6:B:704:GLN:HG3	27:B:848:DGD:HA31	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:733:PHE:CD2	12:H:144:PRO:HG2	2.52	0.44
18:B:839:CLA:HBC3	21:B:847:BCR:C21	2.48	0.44
14:J:12:PRO:O	14:J:16:THR:HG22	2.17	0.44
5:A:705:LYS:HB3	5:A:705:LYS:HE3	1.79	0.44
21:A:849:BCR:H361	21:A:849:BCR:H20C	1.84	0.44
1:1:235:ILE:HB	18:1:612:CLA:H12	1.98	0.44
17:4:605:CHL:HHC	17:4:605:CHL:HBB1	2.00	0.44
5:A:331:THR:HG21	22:A:855:LHG:O1	2.18	0.44
18:A:802:CLA:H92	18:A:802:CLA:H62	1.76	0.44
16:L:204:LEU:HD23	16:L:208:LEU:HD12	1.99	0.44
2:2:173:ASP:HB3	2:2:176:PHE:O	2.18	0.44
2:2:109:GLY:HA2	20:2:616:XAT:H181	2.00	0.44
3:3:229:ILE:HD13	3:3:229:ILE:HA	1.91	0.44
19:3:614:LUT:H181	19:3:614:LUT:H7	1.73	0.44
6:B:15:ASP:OD1	6:B:20:ARG:HB2	2.17	0.44
22:1:621:LHG:HC62	22:1:621:LHG:H241	1.40	0.44
21:A:847:BCR:H24C	21:A:847:BCR:H371	1.83	0.43
21:B:842:BCR:H24C	21:B:842:BCR:H371	1.89	0.43
18:B:807:CLA:H102	18:B:807:CLA:H61	1.86	0.43
18:B:809:CLA:H152	18:B:809:CLA:H112	1.59	0.43
21:F:302:BCR:H24C	21:F:302:BCR:H371	1.85	0.43
18:1:603:CLA:H92	18:1:603:CLA:H62	1.81	0.43
18:A:817:CLA:H2	18:K:202:CLA:HED1	2.01	0.43
4:4:220:PHE:HE1	19:4:616:LUT:H41	1.84	0.43
5:A:717:LEU:HB3	5:A:721:GLN:HG2	1.99	0.43
21:G:205:BCR:H24C	21:G:205:BCR:H371	1.80	0.43
14:J:33:PHE:CD1	21:J:101:BCR:H312	2.54	0.43
1:1:114:TRP:H	1:1:114:TRP:CD1	2.37	0.43
18:F:301:CLA:H61	18:F:301:CLA:H41	1.77	0.43
21:J:101:BCR:H393	21:J:101:BCR:H24C	1.71	0.43
22:2:617:LHG:H291	22:2:617:LHG:HC91	2.01	0.43
5:A:213:HIS:CD2	5:A:213:HIS:C	2.97	0.43
18:B:804:CLA:HBA1	18:B:804:CLA:H3A	1.76	0.43
10:F:125:GLU:HA	10:F:125:GLU:OE2	2.19	0.43
6:B:91:ILE:HB	6:B:112:PRO:HB2	2.01	0.43
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.54	0.43
18:B:838:CLA:H92	18:B:838:CLA:H61	1.84	0.43
4:4:194:LEU:HD12	19:4:616:LUT:H222	2.01	0.43
18:H:201:CLA:HBC1	21:L:306:BCR:H352	2.01	0.43
21:1:617:BCR:H24C	21:1:617:BCR:H371	1.90	0.43
19:3:614:LUT:H35	19:3:614:LUT:H401	1.79	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:3:617:CLA:HED1	5:A:181:ALA:HB1	2.00	0.43
5:A:703:HIS:HB3	5:A:708:VAL:O	2.19	0.43
21:A:850:BCR:H24C	21:A:850:BCR:H371	1.79	0.43
5:A:693:GLN:O	5:A:697:GLU:HG3	2.18	0.42
6:B:411:MET:HE1	18:B:829:CLA:C3C	2.48	0.42
22:1:621:LHG:HC5	22:1:621:LHG:HC81	1.38	0.42
4:4:113:LEU:HB3	4:4:114:PRO:HD3	2.00	0.42
4:4:237:GLN:HE21	4:4:237:GLN:HB2	1.65	0.42
18:A:807:CLA:H3A	18:A:830:CLA:HAB	2.01	0.42
6:B:586:THR:O	6:B:590:VAL:HG13	2.19	0.42
18:B:838:CLA:HBB2	25:B:841:PQN:H141	2.00	0.42
18:B:839:CLA:HBC2	25:B:841:PQN:H201	2.00	0.42
3:3:55:SER:O	3:3:59:LEU:HD12	2.19	0.42
4:4:225:ASN:OD1	4:4:225:ASN:C	2.61	0.42
5:A:296:LEU:O	5:A:300:ILE:HG12	2.18	0.42
5:A:505:LEU:HD11	5:A:513:VAL:HG23	2.00	0.42
1:1:164:PRO:HA	1:1:167:LYS:HD2	2.01	0.42
18:A:830:CLA:H62	18:A:830:CLA:H41	1.82	0.42
5:A:708:VAL:CG1	10:F:180:ARG:HG3	2.49	0.42
16:L:176:LYS:HD3	16:L:176:LYS:HA	1.70	0.42
19:4:616:LUT:H31	19:4:616:LUT:H391	1.95	0.42
24:A:856:LMT:H3'	24:A:856:LMT:H1B	1.76	0.42
14:J:36:ALA:HB1	21:J:101:BCR:C10	2.48	0.42
21:2:618:BCR:H23C	21:2:618:BCR:H383	2.02	0.42
18:A:829:CLA:H92	18:A:829:CLA:H61	1.94	0.42
21:A:845:BCR:H371	21:A:845:BCR:H24C	1.87	0.42
18:B:816:CLA:H3A	18:B:816:CLA:HBA2	1.84	0.42
23:B:849:LMG:H111	23:B:849:LMG:HC8	1.35	0.42
1:1:97:MET:SD	18:1:609:CLA:HBB1	2.59	0.42
21:2:618:BCR:H373	21:2:618:BCR:H19C	2.02	0.42
17:4:605:CHL:HBB2	17:4:606:CHL:CBB	2.47	0.42
18:A:806:CLA:HBA1	18:A:806:CLA:H3A	1.74	0.42
21:K:204:BCR:H392	21:K:204:BCR:H24C	1.69	0.42
18:2:609:CLA:H61	18:2:609:CLA:H41	1.86	0.42
23:B:849:LMG:HC92	23:B:849:LMG:H291	1.55	0.42
8:D:153:ASN:OD1	8:D:153:ASN:C	2.63	0.42
18:1:614:CLA:HBA1	19:1:619:LUT:H41	2.02	0.42
18:A:831:CLA:HMA2	16:L:72:THR:HG21	2.01	0.42
5:A:28:ARG:HA	5:A:29:PRO:HD3	1.91	0.41
21:B:842:BCR:H20C	21:B:842:BCR:H361	1.90	0.41
7:C:39:ILE:HG12	7:C:40:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:171:LEU:HD12	5:A:171:LEU:HA	1.95	0.41
5:A:531:PHE:HZ	21:A:850:BCR:H322	1.83	0.41
6:B:26:ALA:HB2	27:B:848:DGD:HA41	2.01	0.41
6:B:668:ARG:HD2	6:B:700:LEU:O	2.19	0.41
9:E:87:VAL:HG11	9:E:138:ILE:HD11	2.02	0.41
18:K:202:CLA:HBA1	18:K:202:CLA:HBD	2.02	0.41
6:B:456:GLU:HA	6:B:457:PRO:HD3	1.94	0.41
10:F:199:ILE:HD11	14:J:14:LEU:HD23	2.02	0.41
18:1:608:CLA:H2	18:1:608:CLA:H62	1.96	0.41
19:1:615:LUT:H15	19:1:615:LUT:H201	1.95	0.41
5:A:688:GLY:HA3	6:B:569:ASP:HB2	2.02	0.41
18:B:813:CLA:H141	18:B:813:CLA:H162	1.89	0.41
7:C:23:THR:HG21	7:C:47:ASP:O	2.21	0.41
9:E:86:LYS:HA	9:E:86:LYS:HD3	1.80	0.41
18:2:604:CLA:HBA2	18:2:604:CLA:H122	2.03	0.41
3:3:86:PRO:HA	3:3:89:LEU:HD12	2.01	0.41
3:3:219:ILE:O	3:3:223:ARG:HG3	2.20	0.41
18:4:601:CLA:HBB2	18:4:602:CLA:HBC2	2.02	0.41
21:A:845:BCR:H23C	21:A:845:BCR:H403	2.02	0.41
6:B:226:PHE:CE1	18:G:203:CLA:HBC1	2.56	0.41
16:L:142:LEU:HD22	21:L:305:BCR:H401	2.02	0.41
18:1:612:CLA:HAA1	18:1:612:CLA:HBD	2.01	0.41
18:A:809:CLA:H41	18:A:809:CLA:H62	1.86	0.41
18:2:610:CLA:HBC3	22:2:617:LHG:HC62	2.03	0.41
3:3:83:PHE:HD2	18:3:603:CLA:H52	1.84	0.41
3:3:119:ILE:HG13	3:3:120:PRO:HD2	2.01	0.41
3:3:153:LEU:HD12	3:3:153:LEU:HA	1.86	0.41
21:3:601:BCR:H24C	21:3:601:BCR:H371	1.90	0.41
5:A:205:LEU:HD13	21:A:846:BCR:H20C	2.02	0.41
18:B:816:CLA:HBB1	18:B:816:CLA:HHC	2.03	0.41
18:H:201:CLA:HAC2	18:L:302:CLA:HAA2	2.03	0.41
19:1:619:LUT:H15	19:1:619:LUT:H201	1.86	0.41
3:3:179:LEU:HD23	3:3:179:LEU:HA	1.86	0.41
21:A:845:BCR:H383	21:K:204:BCR:H10C	2.01	0.41
21:2:618:BCR:H24C	21:2:618:BCR:H403	1.79	0.41
3:3:229:ILE:HG21	20:3:615:XAT:H14	2.03	0.41
5:A:455:HIS:CD2	5:A:455:HIS:C	2.98	0.41
18:A:802:CLA:H91	18:A:802:CLA:H111	1.86	0.41
18:B:801:CLA:H8	18:B:801:CLA:H51	1.75	0.41
18:B:815:CLA:HHC	18:B:815:CLA:HBB1	2.03	0.41
21:B:843:BCR:H20C	21:B:843:BCR:H361	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:4:LEU:HD23	13:I:4:LEU:HA	1.85	0.41
21:L:307:BCR:H24C	21:L:307:BCR:H371	1.87	0.41
18:A:836:CLA:HHC	18:A:836:CLA:HBB1	2.02	0.41
21:F:305:BCR:H20C	21:F:305:BCR:H361	1.90	0.41
15:K:115:MET:HE2	15:K:119:ILE:HD11	2.02	0.41
18:2:609:CLA:H92	18:2:609:CLA:H62	1.83	0.40
18:A:818:CLA:H92	18:A:818:CLA:H62	1.95	0.40
6:B:422:LEU:HD13	6:B:532:LEU:HA	2.03	0.40
15:K:101:THR:HG22	15:K:102:LEU:H	1.86	0.40
18:1:609:CLA:H62	18:1:609:CLA:H41	1.88	0.40
3:3:66:ASP:OD1	3:3:66:ASP:N	2.52	0.40
4:4:171:ASP:HB3	4:4:174:PHE:O	2.21	0.40
5:A:232:LYS:HA	5:A:232:LYS:HD3	1.58	0.40
6:B:65:LEU:HD11	21:B:844:BCR:H281	2.02	0.40
18:B:823:CLA:H111	18:B:823:CLA:H72	1.97	0.40
12:H:138:LEU:HD23	12:H:138:LEU:HA	1.91	0.40
17:4:605:CHL:H41	17:4:605:CHL:H62	1.78	0.40
18:A:825:CLA:HBD	18:A:825:CLA:HAA2	2.02	0.40
18:A:843:CLA:H162	18:A:843:CLA:H203	1.79	0.40
18:B:813:CLA:HBB2	18:B:827:CLA:H143	2.02	0.40
21:2:618:BCR:HC7	21:2:618:BCR:H10C	1.87	0.40
18:A:817:CLA:H11	15:K:121:LEU:HD22	2.03	0.40
18:B:817:CLA:HBA2	18:B:817:CLA:H3A	1.67	0.40
18:B:823:CLA:HBD	18:B:823:CLA:HAA2	2.04	0.40
1:1:168:LYS:HE2	1:1:168:LYS:HB2	1.71	0.40
2:2:59:LEU:HD11	2:2:66:PRO:HD3	2.03	0.40
21:A:850:BCR:H20C	21:A:850:BCR:H361	1.86	0.40
18:L:302:CLA:HAA1	18:L:302:CLA:HBD	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	192/200 (96%)	190 (99%)	2 (1%)	0	100	100
2	2	201/211 (95%)	196 (98%)	5 (2%)	0	100	100
3	3	211/232 (91%)	207 (98%)	4 (2%)	0	100	100
4	4	196/200 (98%)	189 (96%)	7 (4%)	0	100	100
5	A	722/750 (96%)	706 (98%)	16 (2%)	0	100	100
6	B	731/734 (100%)	712 (97%)	19 (3%)	0	100	100
7	C	78/81 (96%)	70 (90%)	8 (10%)	0	100	100
8	D	138/155 (89%)	128 (93%)	10 (7%)	0	100	100
9	E	61/93 (66%)	59 (97%)	2 (3%)	0	100	100
10	F	153/159 (96%)	147 (96%)	6 (4%)	0	100	100
11	G	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
12	H	92/95 (97%)	90 (98%)	2 (2%)	0	100	100
13	I	30/36 (83%)	30 (100%)	0	0	100	100
14	J	38/42 (90%)	36 (95%)	2 (5%)	0	100	100
15	K	51/84 (61%)	51 (100%)	0	0	100	100
16	L	150/170 (88%)	145 (97%)	5 (3%)	0	100	100
All	All	3140/3342 (94%)	3048 (97%)	92 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	155/160 (97%)	154 (99%)	1 (1%)	78	89
2	2	164/169 (97%)	161 (98%)	3 (2%)	51	74
3	3	166/181 (92%)	162 (98%)	4 (2%)	43	67
4	4	166/167 (99%)	165 (99%)	1 (1%)	78	89
5	A	582/608 (96%)	578 (99%)	4 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	B	597/598 (100%)	591 (99%)	6 (1%)	68	83
7	C	70/71 (99%)	70 (100%)	0	100	100
8	D	119/130 (92%)	117 (98%)	2 (2%)	53	75
9	E	58/79 (73%)	58 (100%)	0	100	100
10	F	128/132 (97%)	127 (99%)	1 (1%)	73	86
11	G	82/83 (99%)	82 (100%)	0	100	100
12	H	79/80 (99%)	79 (100%)	0	100	100
13	I	28/32 (88%)	28 (100%)	0	100	100
14	J	35/37 (95%)	34 (97%)	1 (3%)	37	61
15	K	41/62 (66%)	40 (98%)	1 (2%)	43	67
16	L	118/134 (88%)	117 (99%)	1 (1%)	73	86
All	All	2588/2723 (95%)	2563 (99%)	25 (1%)	65	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	77	GLU
2	2	56	GLU
2	2	77	ASP
2	2	185	ASP
3	3	118	LEU
3	3	121	GLN
3	3	158	PHE
3	3	237	LEU
4	4	127	GLU
5	A	352	LEU
5	A	366	HIS
5	A	392	MET
5	A	457	ASP
6	B	47	PHE
6	B	78	VAL
6	B	257	LEU
6	B	394	PHE
6	B	600	THR
6	B	640	MET
8	D	91	GLU
8	D	131	LEU
10	F	213	ILE

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Mol	Chain	Res	Type
14	J	3	ASP
15	K	115	MET
16	L	214	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	156	GLN
1	1	222	ASN
1	1	232	HIS
1	1	234	ASN
2	2	97	GLN
2	2	231	GLN
3	3	200	ASN
3	3	221	ASN
3	3	235	GLN
4	4	69	ASN
4	4	209	ASN
4	4	237	GLN
4	4	245	ASN
4	4	249	GLN
5	A	113	GLN
5	A	213	HIS
5	A	216	HIS
5	A	243	ASN
5	A	249	GLN
5	A	293	HIS
5	A	307	HIS
5	A	542	HIS
5	A	693	GLN
6	B	10	GLN
6	B	53	GLN
6	B	89	HIS
6	B	114	ASN
6	B	170	ASN
6	B	196	HIS
6	B	210	ASN
6	B	248	GLN
6	B	262	HIS
6	B	299	HIS
6	B	319	HIS
6	B	439	HIS

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Mol	Chain	Res	Type
6	B	467	HIS
6	B	482	ASN
6	B	627	ASN
8	D	157	GLN
8	D	171	ASN
9	E	132	ASN
11	G	130	ASN
12	H	86	ASN
12	H	89	GLN
13	I	29	HIS
15	K	53	ASN
15	K	113	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

215 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	CLA	F	301	-	61,65,73	1.30	7 (11%)	73,103,113	1.73	9 (12%)
21	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	830	6	47,51,73	1.41	8 (17%)	56,86,113	1.85	6 (10%)
18	CLA	B	812	6	69,73,73	1.24	8 (11%)	83,113,113	1.77	12 (14%)
18	CLA	4	612	4	61,65,73	1.30	8 (13%)	73,103,113	1.74	10 (13%)
18	CLA	B	835	-	54,58,73	1.40	7 (12%)	65,95,113	1.89	10 (15%)
18	CLA	A	815	5	46,50,73	1.42	8 (17%)	55,85,113	1.84	6 (10%)
18	CLA	1	608	1	69,73,73	1.22	7 (10%)	83,113,113	1.66	10 (12%)
18	CLA	B	825	6	66,70,73	1.28	8 (12%)	79,109,113	1.74	11 (13%)
18	CLA	H	201	12	55,59,73	1.37	9 (16%)	66,96,113	1.80	11 (16%)
18	CLA	B	814	6	59,63,73	1.34	8 (13%)	71,101,113	1.82	9 (12%)
21	BCR	K	204	-	41,41,41	0.25	0	56,56,56	0.46	0
22	LHG	2	617	-	36,36,48	0.34	0	39,42,54	0.31	0
19	LUT	3	614	-	42,43,43	1.64	8 (19%)	51,60,60	1.82	11 (21%)
18	CLA	A	836	5	49,53,73	1.40	8 (16%)	59,89,113	1.89	9 (15%)
18	CLA	A	806	5	69,73,73	1.24	8 (11%)	83,113,113	1.75	8 (9%)
18	CLA	3	606	-	44,49,73	1.45	7 (15%)	52,84,113	1.83	4 (7%)
18	CLA	B	834	-	46,50,73	1.43	8 (17%)	55,85,113	1.92	7 (12%)
19	LUT	1	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.53	9 (17%)
17	CHL	2	606	-	42,51,74	2.49	14 (33%)	31,86,114	3.37	15 (48%)
18	CLA	1	603	1	59,63,73	1.32	8 (13%)	71,101,113	1.86	10 (14%)
18	CLA	4	614	4	54,58,73	1.39	8 (14%)	65,95,113	1.79	10 (15%)
18	CLA	A	817	5	64,68,73	1.29	8 (12%)	77,107,113	1.69	11 (14%)
21	BCR	A	846	-	41,41,41	0.15	0	56,56,56	0.60	2 (3%)
22	LHG	A	855	18	29,29,48	0.37	0	32,35,54	0.35	0
21	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.66	1 (1%)
18	CLA	B	829	6	47,51,73	1.42	8 (17%)	56,86,113	1.90	7 (12%)
18	CLA	G	204	11	49,53,73	1.42	7 (14%)	59,89,113	1.82	7 (11%)
21	BCR	L	306	-	41,41,41	0.11	0	56,56,56	0.26	0
18	CLA	A	826	-	69,73,73	1.26	8 (11%)	83,113,113	1.67	12 (14%)
21	BCR	A	845	-	41,41,41	0.14	0	56,56,56	0.25	0
18	CLA	B	840	22	69,73,73	1.25	8 (11%)	83,113,113	1.69	12 (14%)
18	CLA	3	610	3	47,51,73	1.42	7 (14%)	56,86,113	1.84	8 (14%)
18	CLA	A	839	5	54,58,73	1.40	8 (14%)	65,95,113	1.84	10 (15%)
18	CLA	4	602	4	64,68,73	1.28	8 (12%)	77,107,113	1.72	12 (15%)
18	CLA	B	826	6	64,68,73	1.27	8 (12%)	77,107,113	1.75	12 (15%)
18	CLA	A	842	-	69,73,73	1.24	7 (10%)	83,113,113	1.70	9 (10%)
23	LMG	4	621	-	49,49,55	0.19	0	57,57,63	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	SF4	C	101	7	0,12,12	-	-	-		
23	LMG	1	620	-	53,53,55	0.18	0	61,61,63	0.16	0
18	CLA	3	604	-	49,53,73	1.42	8 (16%)	59,89,113	1.81	8 (13%)
18	CLA	3	602	3	64,68,73	1.29	8 (12%)	77,107,113	1.73	12 (15%)
17	CHL	4	606	-	45,54,74	2.46	15 (33%)	35,90,114	3.19	16 (45%)
18	CLA	B	810	6	58,62,73	1.34	9 (15%)	73,100,113	2.05	11 (15%)
17	CHL	4	615	4	40,49,74	2.45	12 (30%)	31,84,114	3.27	14 (45%)
18	CLA	A	840	5	69,73,73	1.23	7 (10%)	83,113,113	1.71	11 (13%)
18	CLA	L	303	16	64,68,73	1.28	8 (12%)	77,107,113	1.73	12 (15%)
18	CLA	1	613	1	49,53,73	1.43	8 (16%)	59,89,113	1.88	10 (16%)
18	CLA	3	613	3	43,48,73	1.48	8 (18%)	51,83,113	1.87	8 (15%)
18	CLA	A	804	5	59,63,73	1.33	8 (13%)	71,101,113	1.85	12 (16%)
18	CLA	B	820	6	59,63,73	1.34	8 (13%)	71,101,113	1.74	11 (15%)
18	CLA	B	819	6	54,58,73	1.39	8 (14%)	65,95,113	1.85	10 (15%)
17	CHL	2	614	2	42,51,74	2.46	12 (28%)	31,86,114	3.36	15 (48%)
18	CLA	2	604	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	12 (14%)
18	CLA	A	828	5	69,73,73	1.22	7 (10%)	83,113,113	1.72	9 (10%)
18	CLA	F	304	10	45,49,73	1.46	9 (20%)	54,84,113	1.99	10 (18%)
18	CLA	1	604	-	53,57,73	1.37	7 (13%)	62,93,113	1.86	7 (11%)
19	LUT	1	619	-	42,43,43	1.64	8 (19%)	51,60,60	1.59	11 (21%)
20	XAT	3	615	-	39,47,47	0.09	0	54,74,74	0.79	3 (5%)
21	BCR	J	103	-	41,41,41	0.14	0	56,56,56	0.26	0
21	BCR	1	617	-	41,41,41	0.12	0	56,56,56	0.29	0
21	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.45	0
18	CLA	A	810	5	54,58,73	1.41	8 (14%)	65,95,113	1.75	11 (16%)
18	CLA	1	612	1	69,73,73	1.23	8 (11%)	83,113,113	1.68	11 (13%)
18	CLA	K	202	-	49,53,73	1.42	7 (14%)	59,89,113	1.76	7 (11%)
24	LMT	G	201	-	36,36,36	0.10	0	47,47,47	0.18	0
23	LMG	1	623	-	50,50,55	0.19	0	58,58,63	0.17	0
21	BCR	4	618	-	41,41,41	0.13	0	56,56,56	0.33	0
17	CHL	4	607	-	50,59,74	2.34	14 (28%)	41,96,114	3.09	19 (46%)
18	CLA	A	832	5	60,64,73	1.32	8 (13%)	72,102,113	1.74	10 (13%)
18	CLA	J	102	-	46,50,73	1.42	7 (15%)	55,85,113	1.89	9 (16%)
18	CLA	A	841	5	69,73,73	1.24	8 (11%)	83,113,113	1.68	10 (12%)
18	CLA	4	613	4	49,53,73	1.42	8 (16%)	59,89,113	1.83	8 (13%)
18	CLA	B	833	6	64,68,73	1.28	8 (12%)	77,107,113	1.71	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	3	607	3	49,53,73	1.42	8 (16%)	59,89,113	1.86	9 (15%)
18	CLA	A	831	5	54,58,73	1.41	8 (14%)	65,95,113	1.88	9 (13%)
18	CLA	A	838	5	59,63,73	1.34	8 (13%)	71,101,113	1.76	8 (11%)
24	LMT	4	620	-	36,36,36	0.11	0	47,47,47	0.16	0
18	CLA	3	608	3	49,53,73	1.42	8 (16%)	59,89,113	1.84	7 (11%)
18	CLA	B	836	6	69,73,73	1.24	8 (11%)	83,113,113	1.67	10 (12%)
18	CLA	A	816	-	49,53,73	1.42	8 (16%)	59,89,113	1.90	5 (8%)
18	CLA	B	839	6	69,73,73	1.23	8 (11%)	83,113,113	1.73	11 (13%)
18	CLA	A	834	5	69,73,73	1.24	8 (11%)	83,113,113	1.74	9 (10%)
18	CLA	B	801	6	69,73,73	1.23	8 (11%)	83,113,113	1.66	11 (13%)
21	BCR	F	305	-	41,41,41	0.12	0	56,56,56	0.31	0
18	CLA	A	854	22	54,58,73	1.41	7 (12%)	65,95,113	1.75	10 (15%)
23	LMG	F	306	-	47,47,55	0.21	0	55,55,63	0.21	0
18	CLA	2	613	2	47,51,73	1.41	8 (17%)	56,86,113	1.87	8 (14%)
18	CLA	B	813	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	9 (10%)
18	CLA	A	809	5	59,63,73	1.33	8 (13%)	71,101,113	1.77	10 (14%)
18	CLA	3	609	3	45,49,73	1.45	7 (15%)	54,84,113	1.84	9 (16%)
18	CLA	4	609	4	58,62,73	1.34	8 (13%)	69,99,113	1.80	10 (14%)
18	CLA	B	822	6	64,68,73	1.29	9 (14%)	77,107,113	1.63	13 (16%)
18	CLA	B	805	6	69,73,73	1.23	8 (11%)	83,113,113	1.77	9 (10%)
17	CHL	3	616	-	46,55,74	2.40	14 (30%)	36,91,114	3.27	17 (47%)
18	CLA	B	815	6	59,63,73	1.33	8 (13%)	71,101,113	1.80	9 (12%)
18	CLA	A	805	5	49,53,73	1.43	8 (16%)	59,89,113	1.92	7 (11%)
21	BCR	J	101	-	41,41,41	0.28	0	56,56,56	0.65	1 (1%)
17	CHL	2	607	-	50,59,74	2.34	15 (30%)	41,96,114	3.05	18 (43%)
21	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.28	0
18	CLA	1	609	1	63,67,73	1.30	7 (11%)	76,106,113	1.72	9 (11%)
18	CLA	A	807	5	69,73,73	1.24	8 (11%)	83,113,113	1.74	12 (14%)
18	CLA	B	823	-	69,73,73	1.23	8 (11%)	83,113,113	1.71	13 (15%)
18	CLA	3	605	-	51,55,73	1.39	7 (13%)	61,91,113	1.88	10 (16%)
18	CLA	B	806	6	56,60,73	1.38	8 (14%)	67,97,113	1.82	10 (14%)
18	CLA	B	838	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
20	XAT	1	616	-	39,47,47	0.11	0	54,74,74	0.81	3 (5%)
18	CLA	3	611	3	47,52,73	1.44	8 (17%)	56,88,113	1.75	7 (12%)
17	CHL	2	605	-	41,50,74	2.49	13 (31%)	30,85,114	3.33	13 (43%)
23	LMG	F	307	-	30,30,55	0.21	0	38,38,63	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	B	816	-	63,67,73	1.29	7 (11%)	75,105,113	1.71	9 (12%)
21	BCR	B	847	-	41,41,41	0.13	0	56,56,56	0.32	0
18	CLA	A	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.75	11 (13%)
23	LMG	4	619	-	36,36,55	0.20	0	44,44,63	0.17	0
18	CLA	F	303	-	46,50,73	1.43	7 (15%)	55,85,113	1.88	7 (12%)
18	CLA	B	817	6	64,68,73	1.28	8 (12%)	77,107,113	1.76	13 (16%)
18	CLA	A	833	5	69,73,73	1.23	8 (11%)	83,113,113	1.70	9 (10%)
18	CLA	2	612	-	59,63,73	1.33	8 (13%)	71,101,113	1.87	12 (16%)
21	BCR	K	205	-	41,41,41	0.11	0	56,56,56	0.21	0
18	CLA	A	843	-	69,73,73	1.23	7 (10%)	83,113,113	1.70	11 (13%)
18	CLA	2	611	2	49,53,73	1.42	8 (16%)	59,89,113	1.88	9 (15%)
21	BCR	F	302	-	41,41,41	0.16	0	56,56,56	0.36	0
27	DGD	B	848	-	62,62,67	0.16	0	76,76,81	0.16	0
18	CLA	B	803	6	45,49,73	1.45	7 (15%)	54,84,113	1.85	9 (16%)
21	BCR	2	618	-	41,41,41	0.27	0	56,56,56	0.59	1 (1%)
20	XAT	4	617	-	39,47,47	0.13	0	54,74,74	0.90	3 (5%)
18	CLA	A	824	5	59,63,73	1.34	8 (13%)	71,101,113	1.70	10 (14%)
21	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.35	0
18	CLA	G	203	11	46,50,73	1.41	8 (17%)	55,85,113	1.92	6 (10%)
18	CLA	1	607	-	47,52,73	1.44	8 (17%)	56,88,113	1.78	7 (12%)
18	CLA	2	608	2	49,53,73	1.43	8 (16%)	59,89,113	1.78	7 (11%)
21	BCR	L	301	-	41,41,41	0.13	0	56,56,56	0.26	0
18	CLA	3	612	-	43,48,73	1.49	8 (18%)	51,83,113	1.75	8 (15%)
18	CLA	K	203	15	50,54,73	1.40	7 (14%)	60,90,113	1.88	8 (13%)
18	CLA	B	832	6	49,53,73	1.42	6 (12%)	59,89,113	1.84	8 (13%)
25	PQN	A	844	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
21	BCR	G	205	-	41,41,41	0.11	0	56,56,56	0.34	0
18	CLA	A	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.68	11 (13%)
18	CLA	L	304	-	49,53,73	1.43	8 (16%)	59,89,113	1.92	9 (15%)
18	CLA	A	811	5	69,73,73	1.24	8 (11%)	83,113,113	1.71	12 (14%)
18	CLA	A	837	5	55,59,73	1.37	8 (14%)	66,96,113	1.97	9 (13%)
24	LMT	A	856	-	36,36,36	0.13	0	47,47,47	0.52	0
24	LMT	A	853	-	36,36,36	0.11	0	47,47,47	0.24	0
18	CLA	B	831	-	69,73,73	1.26	9 (13%)	83,113,113	1.77	12 (14%)
18	CLA	B	824	-	54,58,73	1.40	8 (14%)	65,95,113	1.73	10 (15%)
21	BCR	3	601	-	41,41,41	0.11	0	56,56,56	0.27	0
18	CLA	A	813	5	69,73,73	1.24	8 (11%)	83,113,113	1.78	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	4	610	-	64,68,73	1.29	7 (10%)	77,107,113	1.69	10 (12%)
18	CLA	1	610	22	59,63,73	1.34	7 (11%)	71,101,113	1.78	10 (14%)
18	CLA	B	811	6	47,51,73	1.40	7 (14%)	56,86,113	1.85	7 (12%)
18	CLA	B	828	6	60,64,73	1.34	8 (13%)	72,102,113	1.76	9 (12%)
18	CLA	2	609	2	59,63,73	1.32	8 (13%)	71,101,113	1.77	7 (9%)
18	CLA	B	837	6	51,55,73	1.38	7 (13%)	61,91,113	1.92	10 (16%)
18	CLA	A	822	5	46,50,73	1.43	8 (17%)	55,85,113	1.80	8 (14%)
19	LUT	2	615	-	42,43,43	1.66	8 (19%)	51,60,60	1.52	10 (19%)
21	BCR	B	842	-	41,41,41	0.14	0	56,56,56	0.29	0
18	CLA	B	809	-	69,73,73	1.24	8 (11%)	83,113,113	1.61	10 (12%)
18	CLA	A	829	5	69,73,73	1.23	8 (11%)	83,113,113	1.70	10 (12%)
21	BCR	A	847	-	41,41,41	0.14	0	56,56,56	0.54	1 (1%)
18	CLA	A	823	5	45,49,73	1.46	8 (17%)	54,84,113	1.92	9 (16%)
22	LHG	1	618	18	48,48,48	0.29	0	51,54,54	0.30	0
20	XAT	2	616	-	39,47,47	0.11	0	54,74,74	0.83	4 (7%)
17	CHL	2	601	2	46,55,74	2.44	14 (30%)	36,91,114	3.20	17 (47%)
18	CLA	4	608	4	49,53,73	1.42	8 (16%)	59,89,113	1.91	6 (10%)
17	CHL	1	601	1	54,63,74	2.24	15 (27%)	46,101,114	2.78	16 (34%)
21	BCR	L	307	-	41,41,41	0.12	0	56,56,56	0.25	0
25	PQN	B	841	-	34,34,34	0.26	0	42,45,45	0.52	1 (2%)
18	CLA	A	827	5	69,73,73	1.24	8 (11%)	83,113,113	1.77	10 (12%)
22	LHG	1	621	-	48,48,48	0.30	0	51,54,54	0.31	0
18	CLA	2	610	-	45,49,73	1.46	7 (15%)	54,84,113	1.84	8 (14%)
18	CLA	A	818	5	63,67,73	1.29	7 (11%)	75,105,113	1.75	10 (13%)
18	CLA	B	827	6	69,73,73	1.24	8 (11%)	83,113,113	1.69	11 (13%)
18	CLA	L	302	16	49,53,73	1.42	8 (16%)	59,89,113	1.84	8 (13%)
18	CLA	1	605	-	43,48,73	1.42	7 (16%)	52,82,113	1.92	7 (13%)
22	LHG	A	852	-	48,48,48	0.30	0	51,54,54	0.30	0
18	CLA	B	804	6	69,73,73	1.25	8 (11%)	83,113,113	1.77	13 (15%)
21	BCR	L	305	-	41,41,41	0.19	0	56,56,56	0.34	0
18	CLA	3	603	3	59,63,73	1.33	7 (11%)	71,101,113	1.80	10 (14%)
17	CHL	1	606	1	40,49,74	2.53	13 (32%)	29,84,114	3.33	13 (44%)
18	CLA	A	803	-	69,73,73	1.22	7 (10%)	83,113,113	1.70	11 (13%)
18	CLA	A	820	5	49,53,73	1.42	8 (16%)	59,89,113	1.88	7 (11%)
18	CLA	A	819	5	69,73,73	1.24	8 (11%)	83,113,113	1.68	13 (15%)
18	CLA	1	611	1	49,53,73	1.43	8 (16%)	59,89,113	1.91	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	CLA	G	202	-	49,53,73	1.43	8 (16%)	59,89,113	1.85	7 (11%)
18	CLA	A	801	5	69,73,73	1.22	8 (11%)	83,113,113	1.72	11 (13%)
18	CLA	A	830	5	69,73,73	1.25	8 (11%)	83,113,113	1.68	10 (12%)
18	CLA	B	807	-	69,73,73	1.22	7 (10%)	83,113,113	1.71	11 (13%)
19	LUT	4	616	-	42,43,43	1.65	8 (19%)	51,60,60	1.55	9 (17%)
18	CLA	4	601	4	50,54,73	1.40	8 (16%)	60,90,113	1.83	8 (13%)
26	SF4	C	102	7	0,12,12	-	-	-	-	-
18	CLA	4	603	4	49,53,73	1.41	7 (14%)	59,89,113	1.89	9 (15%)
18	CLA	K	201	15	42,45,73	1.53	8 (19%)	50,78,113	1.85	8 (16%)
18	CLA	A	814	5	49,53,73	1.44	8 (16%)	59,89,113	1.87	9 (15%)
18	CLA	B	802	-	69,73,73	1.25	8 (11%)	83,113,113	1.83	13 (15%)
18	CLA	A	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.64	12 (14%)
26	SF4	A	851	6,5	0,12,12	-	-	-	-	-
18	CLA	A	808	5	54,58,73	1.41	8 (14%)	65,95,113	1.84	11 (16%)
21	BCR	B	845	-	41,41,41	0.12	0	56,56,56	0.35	0
23	LMG	B	849	-	52,52,55	0.20	0	60,60,63	0.15	0
18	CLA	B	818	-	59,63,73	1.34	7 (11%)	71,101,113	1.76	11 (15%)
18	CLA	B	821	6	59,63,73	1.34	8 (13%)	71,101,113	1.76	10 (14%)
17	CHL	4	605	-	55,64,74	2.26	15 (27%)	47,102,114	2.84	18 (38%)
21	BCR	B	843	-	41,41,41	0.20	0	56,56,56	0.45	0
18	CLA	B	808	6	59,63,73	1.34	8 (13%)	71,101,113	1.76	9 (12%)
18	CLA	3	617	5	59,63,73	1.34	8 (13%)	71,101,113	1.77	11 (15%)
21	BCR	I	101	-	41,41,41	0.13	0	56,56,56	0.25	0
18	CLA	2	603	2	47,52,73	1.44	8 (17%)	56,88,113	1.81	7 (12%)
22	LHG	1	622	18	37,37,48	0.33	0	40,43,54	0.31	0
18	CLA	4	611	4	44,49,73	1.45	8 (18%)	52,84,113	1.87	5 (9%)
18	CLA	2	602	2	69,73,73	1.24	8 (11%)	83,113,113	1.65	12 (14%)
18	CLA	1	602	1	65,69,73	1.29	8 (12%)	78,108,113	1.73	12 (15%)
18	CLA	1	614	1	49,53,73	1.42	8 (16%)	59,89,113	1.84	8 (13%)
18	CLA	A	812	5	58,62,73	1.35	8 (13%)	69,99,113	1.82	11 (15%)
18	CLA	4	604	-	49,53,73	1.42	7 (14%)	59,89,113	1.82	9 (15%)
18	CLA	A	835	5	49,53,73	1.41	8 (16%)	59,89,113	1.82	9 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	F	301	-	-	11/30/106/115	-
21	BCR	B	846	-	-	3/29/63/63	0/2/2/2
18	CLA	B	830	6	-	3/13/89/115	-
18	CLA	B	812	6	-	19/39/115/115	-
18	CLA	4	612	4	-	17/30/106/115	-
18	CLA	B	835	-	-	5/21/97/115	-
18	CLA	A	815	5	-	5/12/88/115	-
18	CLA	1	608	1	-	18/39/115/115	-
18	CLA	B	825	6	-	12/36/112/115	-
18	CLA	H	201	12	-	14/23/99/115	-
18	CLA	B	814	6	-	10/27/103/115	-
21	BCR	K	204	-	-	3/29/63/63	0/2/2/2
22	LHG	2	617	-	-	6/41/41/53	-
19	LUT	3	614	-	-	2/29/67/67	0/2/2/2
18	CLA	A	836	5	-	6/15/91/115	-
18	CLA	A	806	5	-	22/39/115/115	-
18	CLA	3	606	-	-	3/10/86/115	-
18	CLA	B	834	-	-	1/12/88/115	-
19	LUT	1	615	-	-	1/29/67/67	0/2/2/2
17	CHL	2	606	-	-	4/12/110/137	-
18	CLA	1	603	1	-	6/27/103/115	-
18	CLA	4	614	4	-	8/21/97/115	-
18	CLA	A	817	5	-	16/33/109/115	-
21	BCR	A	846	-	-	5/29/63/63	0/2/2/2
22	LHG	A	855	18	-	6/34/34/53	-
21	BCR	A	850	-	-	7/29/63/63	0/2/2/2
18	CLA	B	829	6	-	6/13/89/115	-
18	CLA	G	204	11	-	5/15/91/115	-
21	BCR	L	306	-	-	2/29/63/63	0/2/2/2
18	CLA	A	826	-	-	11/39/115/115	-
21	BCR	A	845	-	-	4/29/63/63	0/2/2/2
18	CLA	B	840	22	-	25/39/115/115	-
18	CLA	3	610	3	-	6/13/89/115	-
18	CLA	A	839	5	-	10/21/97/115	-
18	CLA	4	602	4	-	8/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	826	6	-	14/33/109/115	-
18	CLA	A	842	-	-	17/39/115/115	-
23	LMG	4	621	-	-	9/44/64/70	0/1/1/1
26	SF4	C	101	7	-	-	0/6/5/5
23	LMG	1	620	-	-	11/48/68/70	0/1/1/1
18	CLA	3	604	-	-	4/15/91/115	-
18	CLA	3	602	3	-	14/33/109/115	-
17	CHL	4	606	-	-	6/15/113/137	-
18	CLA	B	810	6	-	6/25/101/115	-
17	CHL	4	615	4	-	2/10/106/137	-
18	CLA	A	840	5	-	18/39/115/115	-
18	CLA	L	303	16	-	16/33/109/115	-
18	CLA	1	613	1	-	6/15/91/115	-
18	CLA	3	613	3	-	0/8/84/115	-
18	CLA	A	804	5	-	14/27/103/115	-
18	CLA	B	820	6	-	12/27/103/115	-
18	CLA	B	819	6	-	7/21/97/115	-
17	CHL	2	614	2	-	5/12/110/137	-
18	CLA	2	604	-	-	18/39/115/115	-
18	CLA	A	828	5	-	14/39/115/115	-
18	CLA	F	304	10	-	2/10/86/115	-
18	CLA	1	604	-	-	3/20/96/115	-
19	LUT	1	619	-	-	2/29/67/67	0/2/2/2
20	XAT	3	615	-	-	0/31/93/93	0/4/4/4
21	BCR	J	103	-	-	2/29/63/63	0/2/2/2
21	BCR	1	617	-	-	2/29/63/63	0/2/2/2
21	BCR	A	849	-	-	4/29/63/63	0/2/2/2
18	CLA	A	810	5	-	6/21/97/115	-
18	CLA	1	612	1	-	16/39/115/115	-
18	CLA	K	202	-	-	6/15/91/115	-
24	LMT	G	201	-	-	2/21/61/61	0/2/2/2
23	LMG	1	623	-	-	10/45/65/70	0/1/1/1
21	BCR	4	618	-	-	2/29/63/63	0/2/2/2
17	CHL	4	607	-	-	5/21/119/137	-
18	CLA	A	832	5	-	3/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	J	102	-	-	6/12/88/115	-
18	CLA	A	841	5	-	13/39/115/115	-
18	CLA	4	613	4	-	4/15/91/115	-
18	CLA	B	833	6	-	13/33/109/115	-
18	CLA	3	607	3	-	6/15/91/115	-
18	CLA	A	831	5	-	11/21/97/115	-
18	CLA	A	838	5	-	6/27/103/115	-
24	LMT	4	620	-	-	3/21/61/61	0/2/2/2
18	CLA	3	608	3	-	2/15/91/115	-
18	CLA	B	836	6	-	10/39/115/115	-
18	CLA	A	816	-	-	4/15/91/115	-
18	CLA	B	839	6	-	15/39/115/115	-
18	CLA	A	834	5	-	15/39/115/115	-
18	CLA	B	801	6	-	19/39/115/115	-
21	BCR	F	305	-	-	2/29/63/63	0/2/2/2
18	CLA	A	854	22	-	4/21/97/115	-
23	LMG	F	306	-	-	10/42/62/70	0/1/1/1
18	CLA	2	613	2	-	4/13/89/115	-
18	CLA	B	813	6	-	18/39/115/115	-
18	CLA	A	809	5	-	8/27/103/115	-
18	CLA	3	609	3	-	4/10/86/115	-
18	CLA	4	609	4	-	5/26/102/115	-
18	CLA	B	822	6	-	22/33/109/115	-
18	CLA	B	805	6	-	21/39/115/115	-
17	CHL	3	616	-	-	6/17/115/137	-
18	CLA	B	815	6	-	5/27/103/115	-
18	CLA	A	805	5	-	7/15/91/115	-
21	BCR	J	101	-	-	6/29/63/63	0/2/2/2
17	CHL	2	607	-	-	5/21/119/137	-
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
18	CLA	1	609	1	-	7/31/107/115	-
18	CLA	A	807	5	-	16/39/115/115	-
18	CLA	B	823	-	-	13/39/115/115	-
18	CLA	3	605	-	-	6/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	806	6	-	1/24/100/115	-
18	CLA	B	838	-	-	12/39/115/115	-
20	XAT	1	616	-	-	0/31/93/93	0/4/4/4
18	CLA	3	611	3	-	4/13/89/115	-
17	CHL	2	605	-	-	2/10/108/137	-
23	LMG	F	307	-	-	0/25/45/70	0/1/1/1
18	CLA	B	816	-	-	16/32/108/115	-
21	BCR	B	847	-	-	0/29/63/63	0/2/2/2
18	CLA	A	802	-	-	13/39/115/115	-
23	LMG	4	619	-	-	5/31/51/70	0/1/1/1
18	CLA	F	303	-	-	1/12/88/115	-
18	CLA	B	817	6	-	16/33/109/115	-
18	CLA	A	833	5	-	17/39/115/115	-
18	CLA	2	612	-	-	12/27/103/115	-
21	BCR	K	205	-	-	4/29/63/63	0/2/2/2
18	CLA	A	843	-	-	15/39/115/115	-
18	CLA	2	611	2	-	4/15/91/115	-
21	BCR	F	302	-	-	0/29/63/63	0/2/2/2
27	DGD	B	848	-	-	7/50/90/95	0/2/2/2
18	CLA	B	803	6	-	2/10/86/115	-
21	BCR	2	618	-	-	14/29/63/63	0/2/2/2
20	XAT	4	617	-	-	0/31/93/93	0/4/4/4
18	CLA	A	824	5	-	12/27/103/115	-
21	BCR	A	848	-	-	2/29/63/63	0/2/2/2
18	CLA	G	203	11	-	1/12/88/115	-
18	CLA	1	607	-	-	0/13/89/115	-
18	CLA	2	608	2	-	4/15/91/115	-
21	BCR	L	301	-	-	5/29/63/63	0/2/2/2
18	CLA	3	612	-	-	2/8/84/115	-
18	CLA	K	203	15	-	7/17/93/115	-
18	CLA	B	832	6	-	5/15/91/115	-
25	PQN	A	844	-	-	7/23/43/43	0/2/2/2
21	BCR	G	205	-	-	0/29/63/63	0/2/2/2
18	CLA	A	821	-	-	14/39/115/115	-
18	CLA	L	304	-	-	9/15/91/115	-
18	CLA	A	811	5	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	A	837	5	-	10/23/99/115	-
24	LMT	A	856	-	-	5/21/61/61	0/2/2/2
24	LMT	A	853	-	-	4/21/61/61	0/2/2/2
18	CLA	B	831	-	-	16/39/115/115	-
18	CLA	B	824	-	-	5/21/97/115	-
21	BCR	3	601	-	-	0/29/63/63	0/2/2/2
18	CLA	A	813	5	-	17/39/115/115	-
18	CLA	4	610	-	-	11/33/109/115	-
18	CLA	1	610	22	-	4/27/103/115	-
18	CLA	B	811	6	-	2/13/89/115	-
18	CLA	B	828	6	-	11/29/105/115	-
18	CLA	2	609	2	-	3/27/103/115	-
18	CLA	B	837	6	-	6/18/94/115	-
18	CLA	A	822	5	-	4/12/88/115	-
19	LUT	2	615	-	-	1/29/67/67	0/2/2/2
21	BCR	B	842	-	-	0/29/63/63	0/2/2/2
18	CLA	B	809	-	-	18/39/115/115	-
18	CLA	A	829	5	-	16/39/115/115	-
21	BCR	A	847	-	-	3/29/63/63	0/2/2/2
18	CLA	A	823	5	-	3/10/86/115	-
22	LHG	1	618	18	-	11/53/53/53	-
20	XAT	2	616	-	-	0/31/93/93	0/4/4/4
17	CHL	2	601	2	-	4/17/115/137	-
18	CLA	4	608	4	-	3/15/91/115	-
17	CHL	1	601	1	-	10/25/123/137	-
21	BCR	L	307	-	-	4/29/63/63	0/2/2/2
25	PQN	B	841	-	-	7/23/43/43	0/2/2/2
18	CLA	A	827	5	-	13/39/115/115	-
22	LHG	1	621	-	-	13/53/53/53	-
18	CLA	2	610	-	-	1/10/86/115	-
18	CLA	A	818	5	-	9/32/108/115	-
18	CLA	B	827	6	-	17/39/115/115	-
18	CLA	L	302	16	-	6/15/91/115	-
18	CLA	1	605	-	-	2/10/82/115	-
22	LHG	A	852	-	-	11/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	B	804	6	-	15/39/115/115	-
21	BCR	L	305	-	-	3/29/63/63	0/2/2/2
18	CLA	3	603	3	-	8/27/103/115	-
17	CHL	1	606	1	-	3/8/106/137	-
18	CLA	A	803	-	-	9/39/115/115	-
18	CLA	A	820	5	-	3/15/91/115	-
18	CLA	A	819	5	-	20/39/115/115	-
18	CLA	1	611	1	-	5/15/91/115	-
18	CLA	G	202	-	-	7/15/91/115	-
18	CLA	A	801	5	-	11/39/115/115	-
18	CLA	A	830	5	-	15/39/115/115	-
18	CLA	B	807	-	-	14/39/115/115	-
19	LUT	4	616	-	-	1/29/67/67	0/2/2/2
18	CLA	4	601	4	-	6/17/93/115	-
26	SF4	C	102	7	-	-	0/6/5/5
18	CLA	4	603	4	-	6/15/91/115	-
18	CLA	K	201	15	-	0/4/76/115	-
18	CLA	A	814	5	-	3/15/91/115	-
18	CLA	B	802	-	-	17/39/115/115	-
18	CLA	A	825	-	-	20/39/115/115	-
26	SF4	A	851	6,5	-	-	0/6/5/5
18	CLA	A	808	5	-	7/21/97/115	-
21	BCR	B	845	-	-	0/29/63/63	0/2/2/2
23	LMG	B	849	-	-	13/47/67/70	0/1/1/1
18	CLA	B	818	-	-	5/27/103/115	-
18	CLA	B	821	6	-	8/27/103/115	-
17	CHL	4	605	-	-	1/27/125/137	-
21	BCR	B	843	-	-	3/29/63/63	0/2/2/2
18	CLA	B	808	6	-	8/27/103/115	-
18	CLA	3	617	5	-	10/27/103/115	-
21	BCR	I	101	-	-	0/29/63/63	0/2/2/2
18	CLA	2	603	2	-	5/13/89/115	-
22	LHG	1	622	18	-	5/42/42/53	-
18	CLA	4	611	4	-	2/10/86/115	-
18	CLA	2	602	2	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	CLA	1	602	1	-	13/35/111/115	-
18	CLA	1	614	1	-	7/15/91/115	-
18	CLA	A	812	5	-	9/26/102/115	-
18	CLA	4	604	-	-	5/15/91/115	-
18	CLA	A	835	5	-	3/15/91/115	-

All (1319) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	2	606	CHL	CMC-C2C	7.16	1.56	1.44
17	2	601	CHL	C3B-C4B	7.12	1.47	1.41
17	2	605	CHL	CMC-C2C	7.10	1.56	1.44
17	3	616	CHL	CMC-C2C	7.04	1.56	1.44
17	1	606	CHL	CMC-C2C	7.04	1.56	1.44
17	4	605	CHL	CMC-C2C	7.03	1.56	1.44
17	2	601	CHL	CMC-C2C	7.01	1.56	1.44
17	4	606	CHL	CMC-C2C	7.00	1.56	1.44
17	2	614	CHL	CMC-C2C	6.97	1.56	1.44
17	1	601	CHL	CMC-C2C	6.96	1.56	1.44
17	2	607	CHL	CMC-C2C	6.95	1.56	1.44
17	2	606	CHL	C3B-C4B	6.94	1.46	1.41
17	1	606	CHL	C3B-C4B	6.93	1.46	1.41
17	4	615	CHL	CMC-C2C	6.93	1.56	1.44
17	4	606	CHL	C3B-C4B	6.89	1.46	1.41
17	4	607	CHL	C3B-C4B	6.88	1.46	1.41
17	4	607	CHL	CMC-C2C	6.87	1.56	1.44
17	2	614	CHL	C3B-C4B	6.84	1.46	1.41
17	4	605	CHL	C3B-C4B	6.82	1.46	1.41
17	2	605	CHL	C3B-C4B	6.66	1.46	1.41
17	3	616	CHL	C3B-C4B	6.63	1.46	1.41
17	2	607	CHL	C3B-C4B	6.45	1.46	1.41
17	1	601	CHL	C3B-C4B	6.38	1.46	1.41
17	4	615	CHL	C4B-C3B	5.85	1.46	1.39
18	B	831	CLA	MG-NA	5.06	2.18	2.06
18	3	612	CLA	MG-NA	5.04	2.18	2.06
18	3	610	CLA	MG-NA	5.03	2.18	2.06
18	B	812	CLA	MG-NA	5.03	2.18	2.06
18	A	839	CLA	MG-NA	5.03	2.18	2.06
18	B	834	CLA	MG-NA	5.02	2.18	2.06
18	J	102	CLA	MG-NA	5.02	2.18	2.06
18	4	603	CLA	MG-NA	5.02	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	304	CLA	MG-NA	5.02	2.18	2.06
18	B	838	CLA	MG-NA	5.01	2.18	2.06
18	3	603	CLA	MG-NA	5.01	2.18	2.06
18	F	303	CLA	MG-NA	5.00	2.18	2.06
18	G	204	CLA	MG-NA	5.00	2.18	2.06
18	A	825	CLA	MG-NA	5.00	2.18	2.06
18	2	611	CLA	MG-NA	5.00	2.18	2.06
18	3	604	CLA	MG-NA	4.99	2.18	2.06
18	G	202	CLA	MG-NA	4.99	2.18	2.06
18	A	808	CLA	MG-NA	4.98	2.18	2.06
18	B	815	CLA	MG-NA	4.98	2.18	2.06
18	B	808	CLA	MG-NA	4.98	2.18	2.06
18	A	823	CLA	MG-NA	4.98	2.18	2.06
18	3	606	CLA	MG-NA	4.98	2.18	2.06
18	1	605	CLA	MG-NA	4.98	2.18	2.06
18	K	203	CLA	MG-NA	4.98	2.18	2.06
18	3	602	CLA	MG-NA	4.97	2.18	2.06
18	A	854	CLA	MG-NA	4.97	2.18	2.06
18	B	835	CLA	MG-NA	4.97	2.18	2.06
18	3	605	CLA	MG-NA	4.97	2.18	2.06
18	K	201	CLA	MG-NA	4.97	2.18	2.06
18	F	304	CLA	MG-NA	4.97	2.18	2.06
18	4	613	CLA	MG-NA	4.96	2.18	2.06
18	A	841	CLA	MG-NA	4.96	2.18	2.06
18	4	611	CLA	MG-NA	4.96	2.18	2.06
18	1	612	CLA	MG-NA	4.96	2.18	2.06
18	4	614	CLA	MG-NA	4.96	2.18	2.06
18	L	302	CLA	MG-NA	4.96	2.18	2.06
18	A	811	CLA	MG-NA	4.96	2.18	2.06
18	4	604	CLA	MG-NA	4.96	2.18	2.06
18	B	805	CLA	MG-NA	4.96	2.18	2.06
18	B	804	CLA	MG-NA	4.95	2.18	2.06
18	3	607	CLA	MG-NA	4.95	2.18	2.06
18	A	815	CLA	MG-NA	4.95	2.18	2.06
18	K	202	CLA	MG-NA	4.95	2.18	2.06
18	B	814	CLA	MG-NA	4.95	2.18	2.06
18	1	613	CLA	MG-NA	4.95	2.18	2.06
18	B	828	CLA	MG-NA	4.95	2.18	2.06
18	4	612	CLA	MG-NA	4.95	2.18	2.06
18	3	611	CLA	MG-NA	4.95	2.18	2.06
18	2	610	CLA	MG-NA	4.94	2.18	2.06
18	2	613	CLA	MG-NA	4.94	2.18	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	817	CLA	MG-NA	4.94	2.18	2.06
18	A	814	CLA	MG-NA	4.94	2.18	2.06
18	B	829	CLA	MG-NA	4.94	2.18	2.06
18	1	610	CLA	MG-NA	4.94	2.18	2.06
18	A	830	CLA	MG-NA	4.93	2.18	2.06
18	1	602	CLA	MG-NA	4.93	2.18	2.06
18	B	819	CLA	MG-NA	4.93	2.18	2.06
18	2	602	CLA	MG-NA	4.93	2.18	2.06
18	A	843	CLA	MG-NA	4.93	2.18	2.06
18	A	822	CLA	MG-NA	4.93	2.18	2.06
18	A	833	CLA	MG-NA	4.93	2.18	2.06
18	1	611	CLA	MG-NA	4.93	2.18	2.06
18	4	610	CLA	MG-NA	4.93	2.18	2.06
18	A	804	CLA	MG-NA	4.93	2.18	2.06
18	A	831	CLA	MG-NA	4.92	2.18	2.06
18	A	842	CLA	MG-NA	4.92	2.18	2.06
18	2	604	CLA	MG-NA	4.92	2.18	2.06
18	B	823	CLA	MG-NA	4.92	2.18	2.06
18	A	816	CLA	MG-NA	4.92	2.17	2.06
18	2	612	CLA	MG-NA	4.92	2.17	2.06
18	3	613	CLA	MG-NA	4.92	2.17	2.06
18	3	617	CLA	MG-NA	4.92	2.17	2.06
18	1	607	CLA	MG-NA	4.91	2.17	2.06
18	A	813	CLA	MG-NA	4.91	2.17	2.06
18	A	806	CLA	MG-NA	4.91	2.17	2.06
18	B	837	CLA	MG-NA	4.91	2.17	2.06
18	A	838	CLA	MG-NA	4.91	2.17	2.06
18	A	820	CLA	MG-NA	4.90	2.17	2.06
18	1	604	CLA	MG-NA	4.90	2.17	2.06
18	B	810	CLA	MG-NA	4.90	2.17	2.06
18	A	824	CLA	MG-NA	4.90	2.17	2.06
18	A	835	CLA	MG-NA	4.90	2.17	2.06
18	A	805	CLA	MG-NA	4.90	2.17	2.06
18	1	614	CLA	MG-NA	4.89	2.17	2.06
18	B	827	CLA	MG-NA	4.89	2.17	2.06
18	A	837	CLA	MG-NA	4.89	2.17	2.06
18	3	609	CLA	MG-NA	4.89	2.17	2.06
18	B	818	CLA	MG-NA	4.89	2.17	2.06
18	4	602	CLA	MG-NA	4.89	2.17	2.06
18	A	801	CLA	MG-NA	4.88	2.17	2.06
18	A	807	CLA	MG-NA	4.88	2.17	2.06
18	B	833	CLA	MG-NA	4.88	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	F	301	CLA	MG-NA	4.88	2.17	2.06
18	2	603	CLA	MG-NA	4.88	2.17	2.06
18	A	809	CLA	MG-NA	4.88	2.17	2.06
18	B	840	CLA	MG-NA	4.88	2.17	2.06
18	B	806	CLA	MG-NA	4.88	2.17	2.06
18	4	601	CLA	MG-NA	4.88	2.17	2.06
18	A	828	CLA	MG-NA	4.87	2.17	2.06
18	A	812	CLA	MG-NA	4.87	2.17	2.06
18	B	821	CLA	MG-NA	4.87	2.17	2.06
18	2	608	CLA	MG-NA	4.87	2.17	2.06
18	2	609	CLA	MG-NA	4.87	2.17	2.06
18	A	829	CLA	MG-NA	4.87	2.17	2.06
18	B	836	CLA	MG-NA	4.87	2.17	2.06
18	3	608	CLA	MG-NA	4.87	2.17	2.06
18	A	821	CLA	MG-NA	4.87	2.17	2.06
18	G	203	CLA	MG-NA	4.86	2.17	2.06
18	B	839	CLA	MG-NA	4.86	2.17	2.06
18	B	807	CLA	MG-NA	4.86	2.17	2.06
18	B	826	CLA	MG-NA	4.86	2.17	2.06
18	1	603	CLA	MG-NA	4.86	2.17	2.06
18	A	836	CLA	MG-NA	4.86	2.17	2.06
18	B	801	CLA	MG-NA	4.85	2.17	2.06
18	B	809	CLA	MG-NA	4.85	2.17	2.06
18	B	830	CLA	MG-NA	4.85	2.17	2.06
18	A	810	CLA	MG-NA	4.84	2.17	2.06
18	1	609	CLA	MG-NA	4.84	2.17	2.06
18	A	826	CLA	MG-NA	4.84	2.17	2.06
18	4	608	CLA	MG-NA	4.84	2.17	2.06
18	H	201	CLA	MG-NA	4.84	2.17	2.06
18	A	834	CLA	MG-NA	4.84	2.17	2.06
18	A	840	CLA	MG-NA	4.84	2.17	2.06
18	A	827	CLA	MG-NA	4.84	2.17	2.06
18	B	820	CLA	MG-NA	4.83	2.17	2.06
18	A	818	CLA	MG-NA	4.83	2.17	2.06
18	B	813	CLA	MG-NA	4.83	2.17	2.06
18	4	609	CLA	MG-NA	4.82	2.17	2.06
18	A	819	CLA	MG-NA	4.81	2.17	2.06
18	B	817	CLA	MG-NA	4.81	2.17	2.06
18	B	825	CLA	MG-NA	4.81	2.17	2.06
18	1	608	CLA	MG-NA	4.80	2.17	2.06
18	L	303	CLA	MG-NA	4.80	2.17	2.06
18	B	803	CLA	MG-NA	4.79	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	MG-NA	4.79	2.17	2.06
18	A	803	CLA	MG-NA	4.79	2.17	2.06
18	B	822	CLA	MG-NA	4.79	2.17	2.06
18	B	811	CLA	MG-NA	4.78	2.17	2.06
18	B	824	CLA	MG-NA	4.78	2.17	2.06
18	B	816	CLA	MG-NA	4.78	2.17	2.06
18	B	802	CLA	MG-NA	4.77	2.17	2.06
18	A	802	CLA	MG-NA	4.76	2.17	2.06
18	B	832	CLA	MG-NA	4.72	2.17	2.06
17	4	607	CHL	C1C-NC	4.71	1.39	1.35
17	2	605	CHL	C1D-C2D	4.68	1.45	1.39
17	2	614	CHL	C1C-NC	4.65	1.39	1.35
17	1	601	CHL	C1C-NC	4.65	1.39	1.35
17	4	615	CHL	C1C-NC	4.63	1.39	1.35
17	1	606	CHL	C1C-NC	4.63	1.39	1.35
17	2	601	CHL	C1D-C2D	4.61	1.45	1.39
17	2	601	CHL	C1C-NC	4.59	1.39	1.35
17	2	606	CHL	C1D-C2D	4.57	1.45	1.39
17	2	606	CHL	C1C-NC	4.53	1.39	1.35
17	1	601	CHL	C1D-C2D	4.52	1.45	1.39
17	2	614	CHL	C1D-C2D	4.52	1.45	1.39
17	2	605	CHL	C1C-NC	4.51	1.39	1.35
17	4	615	CHL	C1B-C2B	4.51	1.45	1.39
17	1	606	CHL	C1D-C2D	4.48	1.45	1.39
17	4	605	CHL	C1D-C2D	4.48	1.45	1.39
17	3	616	CHL	C1D-C2D	4.46	1.44	1.39
17	2	607	CHL	C1C-NC	4.45	1.39	1.35
17	4	615	CHL	C1D-C2D	4.45	1.44	1.39
17	2	607	CHL	C1D-C2D	4.45	1.44	1.39
17	3	616	CHL	C1B-C2B	4.44	1.44	1.39
17	4	606	CHL	C1D-C2D	4.44	1.44	1.39
17	4	607	CHL	C1D-C2D	4.41	1.44	1.39
17	2	605	CHL	C1B-C2B	4.39	1.44	1.39
17	3	616	CHL	C1C-NC	4.38	1.39	1.35
17	4	606	CHL	C1C-NC	4.36	1.39	1.35
17	2	607	CHL	C1B-C2B	4.32	1.44	1.39
17	1	601	CHL	C1B-C2B	4.30	1.44	1.39
17	2	606	CHL	C1B-C2B	4.29	1.44	1.39
17	4	605	CHL	C1B-C2B	4.29	1.44	1.39
17	4	605	CHL	C1C-NC	4.29	1.39	1.35
17	2	614	CHL	C1B-C2B	4.27	1.44	1.39
17	2	601	CHL	C1B-C2B	4.21	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	606	CHL	C1B-C2B	4.19	1.44	1.39
17	1	606	CHL	C1B-C2B	4.18	1.44	1.39
19	1	615	LUT	C34-C33	4.12	1.41	1.35
19	3	614	LUT	C30-C29	4.10	1.41	1.35
17	4	607	CHL	C1B-C2B	4.10	1.44	1.39
19	2	615	LUT	C34-C33	4.05	1.41	1.35
19	3	614	LUT	C10-C9	4.04	1.41	1.35
19	4	616	LUT	C34-C33	4.02	1.41	1.35
19	2	615	LUT	C14-C13	4.02	1.41	1.35
19	4	616	LUT	C14-C13	4.00	1.41	1.35
19	3	614	LUT	C14-C13	3.99	1.41	1.35
19	1	615	LUT	C30-C29	3.97	1.41	1.35
19	2	615	LUT	C30-C29	3.97	1.41	1.35
19	2	615	LUT	C10-C9	3.96	1.41	1.35
19	1	615	LUT	C10-C9	3.95	1.41	1.35
19	1	619	LUT	C10-C9	3.95	1.41	1.35
19	1	619	LUT	C34-C33	3.94	1.41	1.35
19	1	615	LUT	C14-C13	3.94	1.41	1.35
19	3	614	LUT	C34-C33	3.94	1.41	1.35
19	4	616	LUT	C30-C29	3.90	1.41	1.35
19	4	616	LUT	C10-C9	3.90	1.40	1.35
19	1	619	LUT	C14-C13	3.84	1.40	1.35
19	1	619	LUT	C30-C29	3.81	1.40	1.35
17	4	615	CHL	CAB-C3B	-3.80	1.43	1.51
17	2	606	CHL	C4C-NC	3.77	1.38	1.35
17	2	614	CHL	C4C-NC	3.75	1.38	1.35
17	1	606	CHL	C4C-NC	3.75	1.38	1.35
17	4	615	CHL	C4C-NC	3.72	1.38	1.35
17	4	606	CHL	C4C-NC	3.67	1.38	1.35
17	2	605	CHL	C4C-NC	3.67	1.38	1.35
17	1	601	CHL	C4C-NC	3.66	1.38	1.35
17	2	601	CHL	C4C-NC	3.65	1.38	1.35
17	2	607	CHL	CHA-CBD	3.65	1.55	1.51
17	4	607	CHL	C4C-NC	3.64	1.38	1.35
17	4	605	CHL	C3B-C2B	-3.63	1.35	1.40
17	2	607	CHL	C4C-NC	3.62	1.38	1.35
17	3	616	CHL	CHA-CBD	3.62	1.55	1.51
17	1	606	CHL	CHA-CBD	3.60	1.55	1.51
17	4	606	CHL	C3B-C2B	-3.58	1.35	1.40
17	4	607	CHL	C3B-C2B	-3.58	1.35	1.40
17	3	616	CHL	C4C-NC	3.57	1.38	1.35
17	2	614	CHL	CHA-CBD	3.57	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	4	605	CHL	CHA-CBD	3.56	1.55	1.51
17	4	615	CHL	CHA-CBD	3.55	1.55	1.51
17	4	605	CHL	C4C-NC	3.55	1.38	1.35
17	2	606	CHL	C3B-C2B	-3.53	1.35	1.40
17	2	606	CHL	CHA-CBD	3.53	1.55	1.51
17	4	607	CHL	CHA-CBD	3.53	1.55	1.51
17	1	601	CHL	CHA-CBD	3.53	1.55	1.51
17	2	607	CHL	C3B-C2B	-3.52	1.35	1.40
17	1	601	CHL	C3B-C2B	-3.52	1.35	1.40
17	2	605	CHL	CHA-CBD	3.49	1.55	1.51
17	2	601	CHL	C3B-C2B	-3.49	1.35	1.40
17	2	605	CHL	C3B-C2B	-3.47	1.35	1.40
17	2	614	CHL	O2D-CGD	3.47	1.41	1.33
17	2	605	CHL	O2D-CGD	3.45	1.41	1.33
17	2	601	CHL	CHA-CBD	3.44	1.55	1.51
17	2	606	CHL	O2D-CGD	3.42	1.41	1.33
17	1	606	CHL	C3B-C2B	-3.42	1.35	1.40
17	3	616	CHL	C3B-C2B	-3.42	1.35	1.40
17	4	606	CHL	CHA-CBD	3.40	1.55	1.51
17	1	606	CHL	O2D-CGD	3.39	1.41	1.30
17	4	606	CHL	O2D-CGD	3.38	1.41	1.33
17	4	615	CHL	O2D-CGD	3.37	1.41	1.30
17	4	606	CHL	O2A-CGA	3.36	1.42	1.30
17	4	605	CHL	O2D-CGD	3.36	1.41	1.33
17	3	616	CHL	O2D-CGD	3.36	1.41	1.33
17	2	607	CHL	O2D-CGD	3.33	1.41	1.33
17	2	614	CHL	C3B-C2B	-3.29	1.35	1.40
17	1	601	CHL	O2D-CGD	3.27	1.41	1.30
17	4	607	CHL	O2D-CGD	3.26	1.41	1.33
17	2	601	CHL	O2D-CGD	3.23	1.41	1.33
18	A	810	CLA	C1D-ND	-2.98	1.34	1.37
17	2	607	CHL	O2A-CGA	2.98	1.42	1.33
17	4	605	CHL	O2A-CGA	2.97	1.42	1.33
18	A	802	CLA	C1D-ND	-2.96	1.34	1.37
17	4	607	CHL	O2A-CGA	2.94	1.41	1.33
18	B	802	CLA	C1D-ND	-2.93	1.34	1.37
17	1	601	CHL	O2A-CGA	2.89	1.41	1.33
18	A	826	CLA	C1D-ND	-2.87	1.34	1.37
18	B	825	CLA	C1D-ND	-2.86	1.34	1.37
17	3	616	CHL	O2A-CGA	2.86	1.42	1.33
17	2	607	CHL	C1A-CHA	2.86	1.43	1.40
18	A	806	CLA	C1D-ND	-2.85	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	812	CLA	C1D-ND	-2.84	1.34	1.37
18	B	820	CLA	C1D-ND	-2.83	1.34	1.37
18	B	836	CLA	C1D-ND	-2.83	1.34	1.37
17	2	601	CHL	O2A-CGA	2.83	1.42	1.33
18	B	824	CLA	C1D-ND	-2.83	1.34	1.37
18	B	839	CLA	C1D-ND	-2.82	1.34	1.37
18	B	833	CLA	C1D-ND	-2.82	1.34	1.37
17	3	616	CHL	C1A-CHA	2.81	1.43	1.40
18	A	813	CLA	C1D-ND	-2.81	1.34	1.37
18	1	614	CLA	C1D-ND	-2.81	1.34	1.37
18	F	304	CLA	C1D-ND	-2.81	1.34	1.37
19	1	619	LUT	C8-C9	-2.81	1.39	1.45
18	A	805	CLA	C1D-ND	-2.81	1.34	1.37
19	4	616	LUT	C8-C9	-2.80	1.39	1.45
18	A	834	CLA	C1D-ND	-2.80	1.34	1.37
18	B	804	CLA	C1D-ND	-2.80	1.34	1.37
18	A	827	CLA	C1D-ND	-2.80	1.34	1.37
18	A	840	CLA	C1D-ND	-2.79	1.34	1.37
17	4	605	CHL	C1A-CHA	2.79	1.43	1.40
18	4	608	CLA	C1D-ND	-2.79	1.34	1.37
18	A	841	CLA	C1D-ND	-2.79	1.34	1.37
18	3	602	CLA	C1D-ND	-2.78	1.34	1.37
18	B	813	CLA	C1D-ND	-2.78	1.34	1.37
18	3	608	CLA	C1D-ND	-2.78	1.34	1.37
18	2	608	CLA	C1D-ND	-2.78	1.34	1.37
18	A	843	CLA	C1D-ND	-2.78	1.34	1.37
19	2	615	LUT	C8-C9	-2.78	1.40	1.45
18	2	609	CLA	C1D-ND	-2.77	1.34	1.37
18	B	822	CLA	C1D-ND	-2.77	1.34	1.37
18	A	807	CLA	C1D-ND	-2.77	1.34	1.37
18	B	809	CLA	C1D-ND	-2.77	1.34	1.37
18	B	829	CLA	C1D-ND	-2.77	1.34	1.37
18	A	814	CLA	C1D-ND	-2.77	1.34	1.37
18	B	821	CLA	C1D-ND	-2.76	1.34	1.37
18	G	203	CLA	C1D-ND	-2.76	1.34	1.37
18	B	818	CLA	C1D-ND	-2.76	1.34	1.37
18	A	830	CLA	C1D-ND	-2.76	1.34	1.37
18	B	816	CLA	C1D-ND	-2.76	1.34	1.37
17	2	601	CHL	C1A-CHA	2.75	1.43	1.40
17	4	615	CHL	C1A-CHA	2.75	1.43	1.40
18	B	828	CLA	C1D-ND	-2.75	1.34	1.37
18	A	822	CLA	C1D-ND	-2.75	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	601	CLA	C1D-ND	-2.75	1.34	1.37
18	B	832	CLA	C1D-ND	-2.75	1.34	1.37
18	A	831	CLA	C1D-ND	-2.74	1.34	1.37
18	A	835	CLA	C1D-ND	-2.74	1.34	1.37
18	A	803	CLA	C1D-ND	-2.74	1.34	1.37
18	B	815	CLA	C1D-ND	-2.74	1.34	1.37
18	B	811	CLA	C1D-ND	-2.74	1.34	1.37
18	A	818	CLA	C1D-ND	-2.74	1.34	1.37
18	A	837	CLA	C1D-ND	-2.74	1.34	1.37
18	B	812	CLA	C1D-ND	-2.74	1.34	1.37
18	A	821	CLA	C1D-ND	-2.74	1.34	1.37
17	2	614	CHL	C1A-CHA	2.73	1.43	1.40
18	A	829	CLA	C1D-ND	-2.73	1.34	1.37
18	F	301	CLA	C1D-ND	-2.73	1.34	1.37
17	4	606	CHL	C2C-C3C	2.73	1.38	1.36
18	A	804	CLA	C1D-ND	-2.73	1.34	1.37
18	B	807	CLA	C1D-ND	-2.73	1.34	1.37
18	A	828	CLA	C1D-ND	-2.72	1.34	1.37
18	B	819	CLA	C1D-ND	-2.72	1.34	1.37
19	3	614	LUT	C8-C9	-2.72	1.40	1.45
18	B	840	CLA	C1D-ND	-2.72	1.34	1.37
19	1	615	LUT	C8-C9	-2.72	1.40	1.45
18	B	831	CLA	C1D-ND	-2.72	1.34	1.37
18	B	806	CLA	C1D-ND	-2.72	1.34	1.37
18	B	838	CLA	C1D-ND	-2.71	1.34	1.37
17	1	606	CHL	C1A-CHA	2.71	1.43	1.40
18	1	610	CLA	C1D-ND	-2.71	1.34	1.37
18	3	607	CLA	C1D-ND	-2.71	1.34	1.37
18	4	613	CLA	C1D-ND	-2.71	1.34	1.37
18	4	614	CLA	C1D-ND	-2.71	1.34	1.37
18	2	613	CLA	C1D-ND	-2.70	1.34	1.37
18	1	604	CLA	C1D-ND	-2.70	1.34	1.37
18	1	608	CLA	C1D-ND	-2.70	1.34	1.37
18	4	609	CLA	C1D-ND	-2.70	1.34	1.37
18	A	832	CLA	C1D-ND	-2.70	1.34	1.37
18	L	303	CLA	C1D-ND	-2.70	1.34	1.37
18	1	607	CLA	C1D-ND	-2.70	1.34	1.37
18	A	815	CLA	C1D-ND	-2.70	1.34	1.37
18	A	808	CLA	C1D-ND	-2.70	1.34	1.37
18	G	202	CLA	C1D-ND	-2.70	1.34	1.37
18	B	835	CLA	C1D-ND	-2.69	1.34	1.37
18	1	602	CLA	C1D-ND	-2.69	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	611	CLA	C1D-ND	-2.69	1.34	1.37
18	B	823	CLA	C1D-ND	-2.69	1.34	1.37
18	B	803	CLA	C1D-ND	-2.69	1.34	1.37
18	4	602	CLA	C1D-ND	-2.68	1.34	1.37
18	A	833	CLA	C1D-ND	-2.68	1.34	1.37
18	3	606	CLA	C1D-ND	-2.68	1.34	1.37
18	A	838	CLA	C1D-ND	-2.68	1.34	1.37
18	A	809	CLA	C1D-ND	-2.68	1.34	1.37
18	B	808	CLA	C1D-ND	-2.68	1.34	1.37
18	B	827	CLA	C1D-ND	-2.67	1.34	1.37
18	A	839	CLA	C1D-ND	-2.67	1.34	1.37
18	4	612	CLA	C1D-ND	-2.67	1.34	1.37
18	L	304	CLA	C1D-ND	-2.67	1.34	1.37
18	1	603	CLA	C1D-ND	-2.67	1.34	1.37
18	B	810	CLA	C1D-ND	-2.67	1.34	1.37
18	4	604	CLA	C1D-ND	-2.67	1.34	1.37
18	B	814	CLA	C1D-ND	-2.67	1.34	1.37
18	1	612	CLA	C1D-ND	-2.66	1.34	1.37
18	A	817	CLA	C1D-ND	-2.66	1.34	1.37
18	A	824	CLA	C1D-ND	-2.66	1.34	1.37
18	B	830	CLA	C1D-ND	-2.66	1.34	1.37
18	B	837	CLA	C1D-ND	-2.66	1.34	1.37
18	1	605	CLA	C1D-ND	-2.66	1.34	1.37
18	3	617	CLA	C1D-ND	-2.66	1.34	1.37
18	A	811	CLA	C1D-ND	-2.65	1.34	1.37
18	B	826	CLA	C1D-ND	-2.65	1.34	1.37
18	A	842	CLA	C1D-ND	-2.65	1.34	1.37
18	2	602	CLA	C1D-ND	-2.65	1.34	1.37
18	4	611	CLA	C1D-ND	-2.65	1.34	1.37
18	2	604	CLA	C1D-ND	-2.64	1.34	1.37
18	4	609	CLA	C3B-C4B	2.63	1.48	1.42
17	2	606	CHL	C1A-CHA	2.63	1.43	1.40
18	2	610	CLA	C1D-ND	-2.63	1.34	1.37
18	A	801	CLA	C1D-ND	-2.62	1.34	1.37
18	1	609	CLA	C1D-ND	-2.62	1.34	1.37
18	A	825	CLA	C1D-ND	-2.62	1.34	1.37
18	1	613	CLA	C1D-ND	-2.62	1.34	1.37
18	B	801	CLA	C1D-ND	-2.61	1.34	1.37
18	B	805	CLA	C1D-ND	-2.61	1.34	1.37
18	B	817	CLA	C1D-ND	-2.61	1.34	1.37
18	B	834	CLA	C1D-ND	-2.61	1.34	1.37
18	2	603	CLA	C1D-ND	-2.60	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	610	CLA	C1D-ND	-2.60	1.34	1.37
18	L	302	CLA	C1D-ND	-2.60	1.34	1.37
17	1	601	CHL	C1A-CHA	2.60	1.43	1.40
18	3	609	CLA	C1D-ND	-2.59	1.34	1.37
17	4	606	CHL	C1A-CHA	2.59	1.43	1.40
18	3	605	CLA	C1D-ND	-2.59	1.34	1.37
18	A	820	CLA	C1D-ND	-2.59	1.34	1.37
17	2	605	CHL	C1A-CHA	2.59	1.43	1.40
18	A	816	CLA	C1D-ND	-2.58	1.34	1.37
18	2	612	CLA	C1D-ND	-2.58	1.34	1.37
18	A	836	CLA	C1D-ND	-2.58	1.34	1.37
18	3	613	CLA	C1D-ND	-2.58	1.34	1.37
18	4	603	CLA	C1D-ND	-2.57	1.34	1.37
18	A	823	CLA	C1D-ND	-2.57	1.34	1.37
18	A	826	CLA	C3B-C4B	2.57	1.48	1.42
18	A	819	CLA	C1D-ND	-2.57	1.34	1.37
18	K	203	CLA	C1D-ND	-2.56	1.34	1.37
18	4	609	CLA	CHC-C1C	2.56	1.43	1.38
18	B	820	CLA	C3B-C4B	2.56	1.48	1.42
18	B	832	CLA	C3B-C4B	2.56	1.48	1.42
18	3	604	CLA	C1D-ND	-2.56	1.34	1.37
18	1	609	CLA	C3B-C4B	2.55	1.48	1.42
17	4	605	CHL	C2C-C3C	2.55	1.38	1.36
18	F	303	CLA	C1D-ND	-2.55	1.34	1.37
18	H	201	CLA	C1D-ND	-2.55	1.34	1.37
17	4	605	CHL	C2-C3	2.54	1.39	1.33
18	1	611	CLA	C3B-C4B	2.54	1.48	1.42
18	B	836	CLA	C3B-C4B	2.54	1.48	1.42
18	A	826	CLA	CHC-C1C	2.54	1.43	1.38
18	A	831	CLA	C3B-C4B	2.53	1.48	1.42
18	2	611	CLA	C1D-ND	-2.53	1.34	1.37
18	1	602	CLA	C3B-C4B	2.53	1.48	1.42
18	3	606	CLA	C3B-C4B	2.53	1.48	1.42
17	4	607	CHL	C1A-CHA	2.53	1.42	1.40
18	3	609	CLA	C3B-C4B	2.53	1.48	1.42
18	3	617	CLA	C3B-C4B	2.53	1.48	1.42
18	B	806	CLA	C3B-C4B	2.53	1.48	1.42
17	4	606	CHL	MG-NB	2.52	2.10	2.05
18	3	611	CLA	C1D-ND	-2.52	1.34	1.37
18	A	854	CLA	C3B-C4B	2.51	1.48	1.42
18	J	102	CLA	C1D-ND	-2.51	1.34	1.37
18	B	802	CLA	CHC-C1C	2.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	608	CLA	C3B-C4B	2.51	1.48	1.42
18	B	827	CLA	C3B-C4B	2.51	1.48	1.42
18	3	603	CLA	C1D-ND	-2.51	1.34	1.37
18	2	609	CLA	C3B-C4B	2.51	1.48	1.42
18	3	612	CLA	C3B-C4B	2.51	1.48	1.42
17	2	606	CHL	MG-NB	2.51	2.10	2.05
18	K	202	CLA	C3B-C4B	2.51	1.48	1.42
17	4	607	CHL	MG-NB	2.50	2.10	2.05
18	2	610	CLA	C3B-C4B	2.50	1.48	1.42
18	B	820	CLA	CHC-C1C	2.50	1.43	1.38
18	B	802	CLA	C3B-C4B	2.50	1.48	1.42
18	B	828	CLA	C3B-C4B	2.50	1.48	1.42
18	A	854	CLA	C1D-ND	-2.50	1.34	1.37
18	1	613	CLA	C3B-C4B	2.50	1.48	1.42
18	A	808	CLA	C3B-C4B	2.50	1.48	1.42
18	G	204	CLA	C1D-ND	-2.50	1.34	1.37
18	B	832	CLA	CHC-C1C	2.50	1.43	1.38
18	B	821	CLA	C3B-C4B	2.50	1.48	1.42
18	2	604	CLA	C3B-C4B	2.49	1.48	1.42
18	A	822	CLA	C3B-C4B	2.49	1.48	1.42
18	3	612	CLA	C1D-ND	-2.49	1.34	1.37
17	1	601	CHL	C2-C3	2.49	1.39	1.33
18	A	819	CLA	C3B-C4B	2.49	1.48	1.42
18	A	823	CLA	C3B-C4B	2.49	1.48	1.42
18	B	803	CLA	C3B-C4B	2.49	1.48	1.42
18	B	824	CLA	C3B-C4B	2.49	1.48	1.42
18	F	303	CLA	C3B-C4B	2.49	1.48	1.42
17	2	605	CHL	MG-NB	2.48	2.10	2.05
18	1	602	CLA	CHC-C1C	2.48	1.43	1.38
18	3	610	CLA	C3B-C4B	2.48	1.48	1.42
18	4	602	CLA	C3B-C4B	2.48	1.48	1.42
18	K	201	CLA	C3B-C4B	2.48	1.48	1.42
18	K	202	CLA	C1D-ND	-2.48	1.34	1.37
18	2	602	CLA	C3B-C4B	2.48	1.48	1.42
18	B	822	CLA	C3B-C4B	2.48	1.48	1.42
18	3	610	CLA	C1D-ND	-2.47	1.34	1.37
18	L	304	CLA	C3B-C4B	2.47	1.48	1.42
18	A	819	CLA	CHC-C1C	2.47	1.43	1.38
18	A	829	CLA	C3B-C4B	2.47	1.48	1.42
18	A	824	CLA	C3B-C4B	2.47	1.48	1.42
18	K	201	CLA	C1D-ND	-2.47	1.34	1.37
18	B	822	CLA	CHC-C1C	2.47	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	815	CLA	C3B-C4B	2.47	1.48	1.42
18	A	840	CLA	C3B-C4B	2.47	1.48	1.42
18	A	831	CLA	CHC-C1C	2.47	1.43	1.38
18	4	604	CLA	C3B-C4B	2.46	1.48	1.42
18	4	608	CLA	C3B-C4B	2.46	1.48	1.42
17	4	605	CHL	MG-NB	2.46	2.10	2.05
18	B	821	CLA	CHC-C1C	2.46	1.43	1.38
18	B	830	CLA	C3B-C4B	2.46	1.48	1.42
18	2	611	CLA	C3B-C4B	2.46	1.48	1.42
18	B	829	CLA	C3B-C4B	2.46	1.48	1.42
18	B	840	CLA	C3B-C4B	2.46	1.48	1.42
18	A	830	CLA	C3B-C4B	2.46	1.48	1.42
18	3	617	CLA	CHC-C1C	2.46	1.43	1.38
18	2	613	CLA	C3B-C4B	2.46	1.48	1.42
18	B	825	CLA	CHC-C1C	2.45	1.43	1.38
18	A	820	CLA	C3B-C4B	2.45	1.48	1.42
18	B	809	CLA	C3B-C4B	2.45	1.48	1.42
18	A	814	CLA	C3B-C4B	2.45	1.48	1.42
18	A	821	CLA	C3B-C4B	2.45	1.48	1.42
18	B	835	CLA	C3B-C4B	2.45	1.48	1.42
18	1	614	CLA	C3B-C4B	2.45	1.48	1.42
18	J	102	CLA	C3B-C4B	2.45	1.48	1.42
17	2	607	CHL	C2C-C3C	2.45	1.38	1.36
18	3	605	CLA	C3B-C4B	2.44	1.48	1.42
18	B	806	CLA	CHC-C1C	2.44	1.43	1.38
17	1	606	CHL	C2C-C3C	2.44	1.38	1.36
18	A	834	CLA	C3B-C4B	2.44	1.48	1.42
18	L	302	CLA	C3B-C4B	2.44	1.48	1.42
18	4	610	CLA	C3B-C4B	2.44	1.48	1.42
18	B	834	CLA	C3B-C4B	2.44	1.48	1.42
18	A	812	CLA	C3B-C4B	2.44	1.48	1.42
18	2	608	CLA	CHC-C1C	2.44	1.43	1.38
18	A	805	CLA	C3B-C4B	2.44	1.48	1.42
18	A	802	CLA	CHC-C1C	2.44	1.43	1.38
18	B	836	CLA	CHC-C1C	2.43	1.43	1.38
18	K	203	CLA	C3B-C4B	2.43	1.48	1.42
18	A	838	CLA	C3B-C4B	2.43	1.48	1.42
18	B	831	CLA	C3B-C4B	2.43	1.48	1.42
18	1	610	CLA	C3B-C4B	2.43	1.48	1.42
18	3	602	CLA	C3B-C4B	2.43	1.48	1.42
18	A	813	CLA	C3B-C4B	2.43	1.48	1.42
18	B	827	CLA	CHC-C1C	2.43	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	611	CLA	C3B-C4B	2.43	1.48	1.42
18	A	828	CLA	C3B-C4B	2.43	1.48	1.42
18	H	201	CLA	C3B-C4B	2.43	1.48	1.42
17	1	601	CHL	MG-NB	2.43	2.10	2.05
18	3	609	CLA	CHC-C1C	2.43	1.43	1.38
18	3	613	CLA	C3B-C4B	2.43	1.48	1.42
18	G	204	CLA	C3B-C4B	2.43	1.48	1.42
18	A	830	CLA	CHC-C1C	2.43	1.43	1.38
18	A	822	CLA	CHC-C1C	2.43	1.43	1.38
18	A	840	CLA	CHC-C1C	2.42	1.43	1.38
17	3	616	CHL	MG-NB	2.42	2.10	2.05
18	L	303	CLA	C3B-C4B	2.42	1.48	1.42
17	2	614	CHL	MG-NB	2.42	2.10	2.05
18	1	603	CLA	C3B-C4B	2.42	1.48	1.42
17	2	601	CHL	MG-NB	2.42	2.10	2.05
17	2	607	CHL	MG-NB	2.42	2.10	2.05
18	B	824	CLA	CHC-C1C	2.42	1.43	1.38
18	1	614	CLA	CHC-C1C	2.42	1.43	1.38
18	1	607	CLA	C3B-C4B	2.42	1.48	1.42
18	A	810	CLA	C3B-C4B	2.42	1.48	1.42
18	B	817	CLA	C3B-C4B	2.42	1.48	1.42
18	2	602	CLA	CHC-C1C	2.42	1.43	1.38
18	B	829	CLA	CHC-C1C	2.41	1.43	1.38
18	G	203	CLA	C3B-C4B	2.41	1.48	1.42
18	3	603	CLA	C3B-C4B	2.41	1.48	1.42
18	3	611	CLA	C3B-C4B	2.41	1.48	1.42
18	F	304	CLA	C3B-C4B	2.41	1.48	1.42
18	B	811	CLA	C3B-C4B	2.41	1.48	1.42
18	3	607	CLA	C3B-C4B	2.41	1.48	1.42
18	1	609	CLA	CHC-C1C	2.41	1.43	1.38
18	A	829	CLA	CHC-C1C	2.41	1.43	1.38
18	1	605	CLA	C3B-C4B	2.41	1.48	1.42
18	A	832	CLA	C3B-C4B	2.41	1.48	1.42
18	A	811	CLA	C3B-C4B	2.41	1.48	1.42
18	3	604	CLA	C3B-C4B	2.41	1.48	1.42
18	F	301	CLA	C3B-C4B	2.40	1.48	1.42
18	B	832	CLA	C1B-NB	-2.40	1.34	1.37
18	B	804	CLA	CHC-C1C	2.40	1.43	1.38
18	2	603	CLA	C3B-C4B	2.40	1.48	1.42
18	1	604	CLA	C3B-C4B	2.40	1.48	1.42
18	A	808	CLA	CHC-C1C	2.40	1.43	1.38
18	B	828	CLA	CHC-C1C	2.40	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	608	CLA	C3B-C4B	2.40	1.48	1.42
18	A	827	CLA	C3B-C4B	2.40	1.48	1.42
18	A	806	CLA	C3B-C4B	2.40	1.48	1.42
18	4	608	CLA	CHC-C1C	2.40	1.43	1.38
18	B	814	CLA	C3B-C4B	2.39	1.48	1.42
18	B	804	CLA	C3B-C4B	2.39	1.48	1.42
18	A	809	CLA	C3B-C4B	2.39	1.48	1.42
17	1	606	CHL	MG-NB	2.39	2.10	2.05
18	B	811	CLA	CHC-C1C	2.39	1.43	1.38
18	A	818	CLA	C3B-C4B	2.39	1.48	1.42
18	G	202	CLA	C3B-C4B	2.39	1.48	1.42
18	B	818	CLA	C3B-C4B	2.39	1.48	1.42
19	4	616	LUT	C32-C33	-2.39	1.40	1.45
18	A	829	CLA	CHB-C1B	-2.39	1.34	1.39
18	B	825	CLA	C3B-C4B	2.39	1.48	1.42
18	A	815	CLA	CHC-C1C	2.39	1.43	1.38
18	K	201	CLA	CHC-C1C	2.39	1.43	1.38
18	2	610	CLA	MG-NB	2.39	2.10	2.05
18	A	838	CLA	CHC-C1C	2.39	1.43	1.38
18	B	803	CLA	CHC-C1C	2.39	1.43	1.38
18	B	808	CLA	C3B-C4B	2.39	1.48	1.42
18	A	825	CLA	C3B-C4B	2.39	1.48	1.42
18	A	832	CLA	CHC-C1C	2.38	1.43	1.38
18	2	612	CLA	C3B-C4B	2.38	1.48	1.42
18	A	817	CLA	C3B-C4B	2.38	1.48	1.42
18	4	614	CLA	C3B-C4B	2.38	1.48	1.42
18	A	841	CLA	C3B-C4B	2.38	1.48	1.42
18	B	823	CLA	C3B-C4B	2.38	1.48	1.42
18	B	833	CLA	C3B-C4B	2.38	1.48	1.42
18	A	807	CLA	CHC-C1C	2.38	1.43	1.38
18	A	854	CLA	CHC-C1C	2.38	1.43	1.38
18	3	610	CLA	MG-NB	2.38	2.10	2.05
18	A	816	CLA	C3B-C4B	2.38	1.48	1.42
18	2	604	CLA	CHC-C1C	2.38	1.43	1.38
18	1	611	CLA	CHC-C1C	2.38	1.43	1.38
18	A	802	CLA	C3B-C4B	2.38	1.48	1.42
18	A	807	CLA	C3B-C4B	2.37	1.48	1.42
18	A	854	CLA	MG-NB	2.37	2.10	2.05
19	1	619	LUT	C32-C33	-2.37	1.40	1.45
18	2	610	CLA	CHC-C1C	2.37	1.43	1.38
18	B	830	CLA	CHC-C1C	2.37	1.43	1.38
18	A	814	CLA	CHC-C1C	2.37	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	843	CLA	MG-NB	2.37	2.10	2.05
18	B	801	CLA	C3B-C4B	2.37	1.48	1.42
18	A	824	CLA	CHC-C1C	2.37	1.43	1.38
18	F	301	CLA	CHC-C1C	2.37	1.43	1.38
17	4	615	CHL	MG-NB	2.37	2.10	2.05
18	4	602	CLA	CHC-C1C	2.36	1.43	1.38
18	A	827	CLA	CHC-C1C	2.36	1.43	1.38
18	B	805	CLA	C3B-C4B	2.36	1.48	1.42
18	4	604	CLA	CHC-C1C	2.36	1.43	1.38
18	1	608	CLA	C3B-C4B	2.36	1.48	1.42
18	B	809	CLA	CHC-C1C	2.36	1.43	1.38
18	B	810	CLA	CHC-C1C	2.36	1.43	1.38
18	A	843	CLA	C3B-C4B	2.36	1.48	1.42
18	A	809	CLA	CHC-C1C	2.36	1.43	1.38
17	4	606	CHL	CBA-CGA	2.36	1.56	1.50
18	B	813	CLA	C3B-C4B	2.36	1.48	1.42
18	A	805	CLA	CHC-C1C	2.36	1.43	1.38
18	K	202	CLA	MG-NB	2.36	2.10	2.05
18	2	611	CLA	CHB-C1B	-2.36	1.34	1.39
18	A	842	CLA	C3B-C4B	2.36	1.48	1.42
18	3	602	CLA	CHC-C1C	2.36	1.43	1.38
18	F	303	CLA	CHC-C1C	2.36	1.43	1.38
18	2	613	CLA	CHC-C1C	2.36	1.43	1.38
18	4	603	CLA	C3B-C4B	2.35	1.48	1.42
18	4	601	CLA	C3B-C4B	2.35	1.48	1.42
18	H	201	CLA	CHC-C1C	2.35	1.43	1.38
18	4	603	CLA	MG-NB	2.35	2.10	2.05
18	A	804	CLA	C3B-C4B	2.35	1.48	1.42
18	3	606	CLA	CHC-C1C	2.35	1.43	1.38
18	A	806	CLA	CHC-C1C	2.35	1.43	1.38
18	B	837	CLA	C3B-C4B	2.35	1.48	1.42
18	B	815	CLA	C3B-C4B	2.35	1.48	1.42
18	B	814	CLA	CHB-C1B	-2.35	1.34	1.39
18	A	808	CLA	CHB-C1B	-2.35	1.34	1.39
18	B	812	CLA	C3B-C4B	2.35	1.48	1.42
18	A	810	CLA	CHC-C1C	2.35	1.43	1.38
18	4	603	CLA	CHB-C1B	-2.35	1.34	1.39
18	B	816	CLA	C3B-C4B	2.35	1.48	1.42
18	B	817	CLA	CHC-C1C	2.35	1.43	1.38
18	4	613	CLA	C3B-C4B	2.34	1.48	1.42
18	A	820	CLA	CHB-C1B	-2.34	1.34	1.39
18	4	611	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	611	CLA	CHB-C1B	-2.34	1.34	1.39
18	A	833	CLA	C3B-C4B	2.34	1.48	1.42
18	L	304	CLA	CHC-C1C	2.34	1.43	1.38
19	4	616	LUT	C12-C13	-2.34	1.40	1.45
17	4	607	CHL	C2-C3	2.34	1.39	1.32
18	B	812	CLA	CHC-C1C	2.34	1.43	1.38
18	K	203	CLA	CHC-C1C	2.34	1.43	1.38
18	1	613	CLA	CHC-C1C	2.34	1.43	1.38
18	A	834	CLA	CHC-C1C	2.34	1.43	1.38
18	2	609	CLA	CHC-C1C	2.34	1.43	1.38
18	G	203	CLA	CHC-C1C	2.34	1.43	1.38
18	L	303	CLA	CHC-C1C	2.34	1.43	1.38
18	B	813	CLA	CHC-C1C	2.34	1.43	1.38
18	K	202	CLA	CHC-C1C	2.34	1.43	1.38
18	B	830	CLA	CHB-C1B	-2.34	1.34	1.39
19	1	619	LUT	C12-C13	-2.34	1.40	1.45
18	A	801	CLA	CHC-C1C	2.34	1.43	1.38
19	2	615	LUT	C32-C33	-2.33	1.40	1.45
18	A	812	CLA	CHC-C1C	2.33	1.43	1.38
18	A	818	CLA	CHC-C1C	2.33	1.43	1.38
18	B	818	CLA	CHC-C1C	2.33	1.43	1.38
19	1	615	LUT	C12-C13	-2.33	1.40	1.45
18	3	610	CLA	CHC-C1C	2.33	1.43	1.38
18	A	821	CLA	CHC-C1C	2.33	1.43	1.38
18	A	839	CLA	C3B-C4B	2.33	1.48	1.42
18	B	805	CLA	CHB-C1B	-2.33	1.34	1.39
18	A	814	CLA	CHB-C1B	-2.33	1.34	1.39
18	A	823	CLA	CHC-C1C	2.33	1.43	1.38
18	A	816	CLA	CHB-C1B	-2.33	1.34	1.39
18	1	610	CLA	CHC-C1C	2.33	1.43	1.38
18	B	835	CLA	CHC-C1C	2.33	1.43	1.38
18	K	201	CLA	MG-NB	2.33	2.10	2.05
18	A	803	CLA	C3B-C4B	2.33	1.48	1.42
18	F	304	CLA	CHC-C1C	2.33	1.43	1.38
17	2	606	CHL	C2C-C3C	2.33	1.38	1.36
18	3	603	CLA	MG-NB	2.32	2.10	2.05
18	3	603	CLA	CHB-C1B	-2.32	1.34	1.39
18	B	835	CLA	CHB-C1B	-2.32	1.34	1.39
18	4	610	CLA	MG-NB	2.32	2.10	2.05
18	A	828	CLA	CHC-C1C	2.32	1.43	1.38
18	3	610	CLA	CHB-C1B	-2.32	1.34	1.39
18	3	612	CLA	MG-NB	2.32	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	615	LUT	C28-C29	-2.32	1.41	1.45
18	B	817	CLA	CHB-C1B	-2.32	1.34	1.39
18	B	833	CLA	CHC-C1C	2.32	1.43	1.38
18	A	811	CLA	CHC-C1C	2.32	1.43	1.38
18	B	840	CLA	CHC-C1C	2.32	1.43	1.38
18	A	814	CLA	C1B-NB	-2.32	1.34	1.37
18	B	815	CLA	CHC-C1C	2.32	1.43	1.38
18	A	817	CLA	CHC-C1C	2.31	1.43	1.38
18	B	826	CLA	C3B-C4B	2.31	1.48	1.42
18	A	803	CLA	MG-NB	2.31	2.10	2.05
18	B	831	CLA	CHB-C1B	-2.31	1.34	1.39
19	1	615	LUT	C32-C33	-2.31	1.41	1.45
18	1	603	CLA	CHB-C1B	-2.31	1.34	1.39
18	2	603	CLA	CHC-C1C	2.31	1.43	1.38
18	2	611	CLA	MG-NB	2.31	2.10	2.05
18	A	815	CLA	CHB-C1B	-2.31	1.34	1.39
18	A	823	CLA	MG-NB	2.31	2.10	2.05
18	A	810	CLA	C1B-NB	-2.31	1.34	1.37
18	A	842	CLA	MG-NB	2.31	2.10	2.05
18	B	827	CLA	CHB-C1B	-2.31	1.34	1.39
18	B	831	CLA	MG-NB	2.31	2.10	2.05
19	1	615	LUT	C28-C29	-2.31	1.41	1.45
18	3	612	CLA	CHC-C1C	2.30	1.43	1.38
18	A	816	CLA	CHC-C1C	2.30	1.43	1.38
18	B	805	CLA	CHC-C1C	2.30	1.43	1.38
18	L	304	CLA	CHB-C1B	-2.30	1.34	1.39
18	A	835	CLA	CHC-C1C	2.30	1.43	1.38
18	L	304	CLA	MG-NB	2.30	2.10	2.05
18	A	824	CLA	CHB-C1B	-2.30	1.34	1.39
18	1	612	CLA	CHB-C1B	-2.30	1.34	1.39
18	3	604	CLA	CHB-C1B	-2.30	1.34	1.39
19	4	616	LUT	C28-C29	-2.30	1.41	1.45
18	B	806	CLA	CHB-C1B	-2.30	1.34	1.39
18	A	813	CLA	CHC-C1C	2.30	1.43	1.38
18	B	831	CLA	CHC-C1C	2.30	1.43	1.38
18	G	202	CLA	CHC-C1C	2.30	1.43	1.38
18	B	819	CLA	C3B-C4B	2.30	1.48	1.42
18	A	841	CLA	CHC-C1C	2.30	1.43	1.38
18	G	204	CLA	CHC-C1C	2.30	1.43	1.38
18	F	303	CLA	MG-NB	2.30	2.10	2.05
18	A	835	CLA	C3B-C4B	2.30	1.48	1.42
18	B	808	CLA	CHC-C1C	2.30	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	612	CLA	C3B-C4B	2.30	1.48	1.42
18	A	836	CLA	C3B-C4B	2.30	1.48	1.42
18	B	837	CLA	MG-NB	2.30	2.10	2.05
18	A	831	CLA	CHB-C1B	-2.30	1.34	1.39
18	A	803	CLA	CHC-C1C	2.30	1.43	1.38
18	A	837	CLA	C3B-C4B	2.30	1.48	1.42
18	A	820	CLA	CHC-C1C	2.30	1.43	1.38
18	3	617	CLA	CHB-C1B	-2.30	1.34	1.39
19	2	615	LUT	C12-C13	-2.30	1.41	1.45
18	4	610	CLA	CHB-C1B	-2.30	1.34	1.39
17	2	601	CHL	C2C-C3C	2.30	1.38	1.36
18	A	838	CLA	CHB-C1B	-2.30	1.34	1.39
18	B	834	CLA	MG-NC	2.29	2.11	2.06
17	2	607	CHL	C2-C3	2.29	1.38	1.32
18	3	613	CLA	CHC-C1C	2.29	1.43	1.38
18	A	819	CLA	CHB-C1B	-2.29	1.34	1.39
18	B	801	CLA	CHC-C1C	2.29	1.43	1.38
18	A	823	CLA	CHB-C1B	-2.29	1.34	1.39
18	J	102	CLA	CHC-C1C	2.29	1.43	1.38
18	B	834	CLA	MG-NB	2.29	2.10	2.05
18	1	608	CLA	CHC-C1C	2.29	1.43	1.38
18	G	202	CLA	CHB-C1B	-2.29	1.34	1.39
18	A	834	CLA	CHB-C1B	-2.29	1.34	1.39
18	2	612	CLA	CHC-C1C	2.29	1.43	1.38
18	2	603	CLA	CHB-C1B	-2.29	1.34	1.39
18	4	614	CLA	CHB-C1B	-2.29	1.34	1.39
18	G	204	CLA	CHB-C1B	-2.29	1.34	1.39
18	1	612	CLA	CHC-C1C	2.28	1.43	1.38
18	3	612	CLA	CHB-C1B	-2.28	1.34	1.39
18	3	606	CLA	CHB-C1B	-2.28	1.34	1.39
18	G	204	CLA	MG-NB	2.28	2.10	2.05
18	2	608	CLA	CHB-C1B	-2.28	1.34	1.39
19	1	619	LUT	C28-C29	-2.28	1.41	1.45
18	3	611	CLA	MG-NB	2.28	2.10	2.05
18	B	838	CLA	C3B-C4B	2.28	1.48	1.42
18	3	605	CLA	CHC-C1C	2.28	1.43	1.38
18	1	611	CLA	MG-NB	2.28	2.10	2.05
18	4	604	CLA	CHB-C1B	-2.28	1.34	1.39
18	1	604	CLA	CHC-C1C	2.28	1.43	1.38
18	A	801	CLA	C3B-C4B	2.28	1.48	1.42
18	A	821	CLA	CHB-C1B	-2.28	1.34	1.39
18	3	605	CLA	CHB-C1B	-2.28	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	817	CLA	CHB-C1B	-2.28	1.34	1.39
18	A	825	CLA	CHB-C1B	-2.28	1.34	1.39
18	F	304	CLA	CHB-C1B	-2.28	1.34	1.39
18	1	603	CLA	CHC-C1C	2.28	1.43	1.38
18	4	613	CLA	CHC-C1C	2.28	1.43	1.38
18	4	612	CLA	C3B-C4B	2.28	1.48	1.42
18	4	611	CLA	CHB-C1B	-2.28	1.34	1.39
18	B	823	CLA	CHC-C1C	2.28	1.43	1.38
18	B	840	CLA	CHB-C1B	-2.28	1.34	1.39
18	B	811	CLA	C1B-NB	-2.28	1.35	1.37
18	2	610	CLA	CHB-C1B	-2.28	1.34	1.39
18	B	814	CLA	CHC-C1C	2.28	1.43	1.38
18	A	811	CLA	CHB-C1B	-2.27	1.34	1.39
17	3	616	CHL	C2C-C3C	2.27	1.38	1.36
18	J	102	CLA	MG-NB	2.27	2.10	2.05
18	3	604	CLA	CHC-C1C	2.27	1.43	1.38
18	A	811	CLA	MG-NB	2.27	2.10	2.05
18	B	823	CLA	CHB-C1B	-2.27	1.34	1.39
18	F	303	CLA	CHB-C1B	-2.27	1.34	1.39
18	2	604	CLA	CHB-C1B	-2.27	1.34	1.39
18	J	102	CLA	CHB-C1B	-2.27	1.34	1.39
18	A	812	CLA	CHB-C1B	-2.27	1.34	1.39
18	A	806	CLA	CHB-C1B	-2.27	1.34	1.39
18	A	833	CLA	CHB-C1B	-2.27	1.34	1.39
18	B	838	CLA	CHC-C1C	2.27	1.43	1.38
18	L	302	CLA	CHB-C1B	-2.27	1.34	1.39
18	A	805	CLA	CHB-C1B	-2.26	1.34	1.39
18	B	804	CLA	CHB-C1B	-2.26	1.34	1.39
18	1	609	CLA	CHB-C1B	-2.26	1.34	1.39
18	2	611	CLA	CHC-C1C	2.26	1.43	1.38
18	1	613	CLA	CHB-C1B	-2.26	1.34	1.39
18	A	826	CLA	CHB-C1B	-2.26	1.34	1.39
18	A	828	CLA	CHB-C1B	-2.26	1.34	1.39
18	B	823	CLA	MG-NB	2.26	2.10	2.05
18	B	829	CLA	CHB-C1B	-2.26	1.34	1.39
18	A	841	CLA	CHB-C1B	-2.26	1.34	1.39
18	B	819	CLA	CHC-C1C	2.26	1.43	1.38
18	B	836	CLA	CHB-C1B	-2.26	1.34	1.39
18	B	807	CLA	C3B-C4B	2.26	1.48	1.42
18	L	302	CLA	MG-NB	2.26	2.10	2.05
18	3	608	CLA	CHC-C1C	2.26	1.43	1.38
18	B	834	CLA	CHC-C1C	2.26	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	2	613	CLA	CHB-C1B	-2.26	1.34	1.39
18	A	810	CLA	CHB-C1B	-2.26	1.34	1.39
18	B	828	CLA	CHB-C1B	-2.26	1.34	1.39
18	1	605	CLA	CHC-C1C	2.26	1.43	1.38
18	4	610	CLA	CHC-C1C	2.26	1.43	1.38
18	A	825	CLA	MG-NB	2.25	2.10	2.05
18	A	825	CLA	CHC-C1C	2.25	1.43	1.38
18	A	834	CLA	C1B-NB	-2.25	1.35	1.37
18	B	804	CLA	MG-NB	2.25	2.10	2.05
18	B	807	CLA	MG-NB	2.25	2.10	2.05
18	A	809	CLA	CHB-C1B	-2.25	1.34	1.39
18	B	801	CLA	MG-NB	2.25	2.10	2.05
18	G	202	CLA	MG-NB	2.25	2.10	2.05
18	1	607	CLA	CHC-C1C	2.25	1.43	1.38
18	A	807	CLA	CHB-C1B	-2.25	1.34	1.39
18	B	811	CLA	CHB-C1B	-2.25	1.34	1.39
18	3	605	CLA	MG-NB	2.25	2.10	2.05
18	B	839	CLA	C3B-C4B	2.25	1.48	1.42
18	A	822	CLA	CHB-C1B	-2.25	1.34	1.39
18	4	602	CLA	CHB-C1B	-2.25	1.34	1.39
18	4	614	CLA	CHC-C1C	2.25	1.43	1.38
18	A	842	CLA	CHB-C1B	-2.25	1.34	1.39
18	A	843	CLA	CHC-C1C	2.25	1.43	1.38
18	3	609	CLA	MG-NB	2.25	2.10	2.05
18	B	838	CLA	CHB-C1B	-2.25	1.34	1.39
18	A	839	CLA	CHC-C1C	2.25	1.43	1.38
18	3	606	CLA	MG-NB	2.25	2.10	2.05
18	A	839	CLA	CHB-C1B	-2.25	1.34	1.39
18	A	838	CLA	MG-NB	2.25	2.10	2.05
18	L	302	CLA	CHC-C1C	2.25	1.43	1.38
18	B	839	CLA	CHB-C1B	-2.25	1.34	1.39
18	2	602	CLA	CHB-C1B	-2.25	1.34	1.39
18	B	834	CLA	CHB-C1B	-2.24	1.34	1.39
18	4	601	CLA	CHC-C1C	2.24	1.43	1.38
18	1	605	CLA	CHB-C1B	-2.24	1.34	1.39
18	4	601	CLA	CHB-C1B	-2.24	1.34	1.39
18	1	610	CLA	MG-NB	2.24	2.10	2.05
18	3	611	CLA	CHB-C1B	-2.24	1.34	1.39
18	1	613	CLA	MG-NB	2.24	2.10	2.05
18	B	833	CLA	CHB-C1B	-2.24	1.34	1.39
18	K	203	CLA	MG-NB	2.24	2.10	2.05
18	1	608	CLA	MG-NB	2.24	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	3	610	CLA	MG-NC	2.24	2.11	2.06
18	A	805	CLA	C1B-NB	-2.24	1.35	1.37
18	A	840	CLA	C1B-NB	-2.24	1.35	1.37
18	3	612	CLA	MG-NC	2.24	2.11	2.06
18	4	613	CLA	CHB-C1B	-2.24	1.34	1.39
18	1	603	CLA	MG-NB	2.24	2.10	2.05
18	3	609	CLA	CHB-C1B	-2.24	1.34	1.39
18	A	827	CLA	CHB-C1B	-2.24	1.34	1.39
18	H	201	CLA	CAA-C2A	2.24	1.58	1.54
18	4	611	CLA	MG-NB	2.24	2.10	2.05
18	A	837	CLA	CHC-C1C	2.24	1.43	1.38
18	A	802	CLA	C1B-NB	-2.24	1.35	1.37
18	B	837	CLA	CHC-C1C	2.24	1.43	1.38
18	A	804	CLA	CHB-C1B	-2.24	1.34	1.39
18	3	611	CLA	CHC-C1C	2.24	1.43	1.38
18	A	825	CLA	MG-NC	2.24	2.11	2.06
18	B	810	CLA	CHB-C1B	-2.24	1.34	1.39
17	1	601	CHL	C2C-C3C	2.24	1.38	1.36
18	A	854	CLA	CHB-C1B	-2.23	1.34	1.39
18	H	201	CLA	CHB-C1B	-2.23	1.34	1.39
18	A	819	CLA	MG-NB	2.23	2.10	2.05
18	B	810	CLA	C4B-C3B	2.23	1.48	1.43
18	3	607	CLA	MG-NB	2.23	2.10	2.05
18	1	602	CLA	CHB-C1B	-2.23	1.34	1.39
18	K	203	CLA	CHB-C1B	-2.23	1.34	1.39
18	3	607	CLA	CHC-C1C	2.23	1.43	1.38
18	1	607	CLA	CHB-C1B	-2.23	1.34	1.39
18	B	816	CLA	C1B-NB	-2.23	1.35	1.37
18	1	604	CLA	CHB-C1B	-2.23	1.34	1.39
18	A	817	CLA	MG-NB	2.23	2.10	2.05
18	B	826	CLA	CHC-C1C	2.23	1.43	1.38
18	4	604	CLA	MG-NB	2.23	2.10	2.05
18	B	818	CLA	CHB-C1B	-2.23	1.34	1.39
18	K	202	CLA	MG-NC	2.23	2.11	2.06
18	A	804	CLA	CHC-C1C	2.23	1.43	1.38
18	B	816	CLA	CHB-C1B	-2.23	1.34	1.39
18	B	803	CLA	CHB-C1B	-2.23	1.34	1.39
18	4	608	CLA	MG-NB	2.23	2.10	2.05
18	3	603	CLA	MG-NC	2.23	2.11	2.06
18	A	842	CLA	CHC-C1C	2.23	1.43	1.38
18	B	812	CLA	MG-NC	2.23	2.11	2.06
18	B	821	CLA	CHB-C1B	-2.23	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	608	CLA	CHB-C1B	-2.23	1.34	1.39
18	B	820	CLA	CHB-C1B	-2.23	1.34	1.39
18	A	836	CLA	CHC-C1C	2.23	1.43	1.38
18	A	820	CLA	C1B-NB	-2.23	1.35	1.37
18	A	826	CLA	C1B-NB	-2.23	1.35	1.37
18	B	826	CLA	CHB-C1B	-2.23	1.34	1.39
18	A	823	CLA	MG-NC	2.22	2.11	2.06
19	3	614	LUT	C12-C13	-2.22	1.41	1.45
18	B	835	CLA	MG-NB	2.22	2.10	2.05
18	3	613	CLA	CHB-C1B	-2.22	1.34	1.39
18	B	806	CLA	C1B-NB	-2.22	1.35	1.37
18	2	608	CLA	MG-NB	2.22	2.10	2.05
18	A	829	CLA	C1B-NB	-2.22	1.35	1.37
18	3	603	CLA	CHC-C1C	2.22	1.43	1.38
18	A	816	CLA	MG-NB	2.22	2.10	2.05
18	A	813	CLA	CHB-C1B	-2.22	1.34	1.39
18	B	827	CLA	MG-NB	2.22	2.10	2.05
18	B	825	CLA	C1B-NB	-2.22	1.35	1.37
18	A	813	CLA	C1B-NB	-2.22	1.35	1.37
18	3	604	CLA	MG-NB	2.21	2.10	2.05
17	2	614	CHL	C2C-C3C	2.21	1.38	1.36
18	B	816	CLA	CHC-C1C	2.21	1.43	1.38
18	B	801	CLA	CHB-C1B	-2.21	1.34	1.39
18	B	808	CLA	CHB-C1B	-2.21	1.34	1.39
18	B	831	CLA	MG-NC	2.21	2.11	2.06
18	B	838	CLA	MG-NC	2.21	2.11	2.06
18	K	201	CLA	CHB-C1B	-2.21	1.34	1.39
18	B	803	CLA	MG-NB	2.21	2.10	2.05
18	B	815	CLA	CHB-C1B	-2.21	1.34	1.39
18	A	843	CLA	MG-NC	2.21	2.11	2.06
18	4	608	CLA	CHB-C1B	-2.21	1.34	1.39
18	B	822	CLA	CHB-C1B	-2.21	1.34	1.39
18	A	839	CLA	MG-NB	2.21	2.10	2.05
18	4	609	CLA	CHB-C1B	-2.20	1.34	1.39
18	4	612	CLA	CHC-C1C	2.20	1.43	1.38
18	1	602	CLA	MG-NB	2.20	2.10	2.05
18	2	613	CLA	MG-NB	2.20	2.10	2.05
18	K	201	CLA	MG-NC	2.20	2.11	2.06
18	B	821	CLA	MG-NB	2.20	2.10	2.05
18	A	821	CLA	C1B-NB	-2.20	1.35	1.37
18	A	808	CLA	MG-NB	2.20	2.10	2.05
18	A	833	CLA	MG-NB	2.20	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	1	604	CLA	MG-NB	2.20	2.10	2.05
18	3	608	CLA	MG-NB	2.20	2.10	2.05
18	B	829	CLA	C1B-NB	-2.20	1.35	1.37
18	4	612	CLA	CHB-C1B	-2.20	1.34	1.39
18	4	614	CLA	MG-NC	2.20	2.11	2.06
18	A	837	CLA	CHB-C1B	-2.20	1.34	1.39
18	4	610	CLA	MG-NC	2.20	2.11	2.06
18	3	607	CLA	MG-NC	2.20	2.11	2.06
19	3	614	LUT	C32-C33	-2.20	1.41	1.45
18	B	820	CLA	C1B-NB	-2.20	1.35	1.37
18	A	836	CLA	MG-NB	2.20	2.10	2.05
18	B	838	CLA	MG-NB	2.20	2.10	2.05
18	3	608	CLA	CHB-C1B	-2.20	1.34	1.39
18	A	840	CLA	CHB-C1B	-2.20	1.34	1.39
18	B	840	CLA	MG-NB	2.19	2.10	2.05
18	1	614	CLA	CHB-C1B	-2.19	1.34	1.39
18	B	812	CLA	CHB-C1B	-2.19	1.34	1.39
18	1	605	CLA	MG-NB	2.19	2.10	2.05
18	1	607	CLA	MG-NB	2.19	2.10	2.05
18	B	823	CLA	C1B-NB	-2.19	1.35	1.37
18	J	102	CLA	MG-NC	2.19	2.11	2.06
18	A	832	CLA	CHB-C1B	-2.19	1.34	1.39
18	A	841	CLA	MG-NB	2.19	2.10	2.05
18	B	824	CLA	CHB-C1B	-2.19	1.34	1.39
18	B	828	CLA	MG-NB	2.19	2.10	2.05
18	K	202	CLA	CHB-C1B	-2.19	1.34	1.39
18	4	603	CLA	MG-NC	2.19	2.11	2.06
18	B	807	CLA	CHB-C1B	-2.19	1.34	1.39
18	A	854	CLA	MG-NC	2.19	2.11	2.06
18	3	607	CLA	CHB-C1B	-2.19	1.34	1.39
18	A	828	CLA	MG-NB	2.19	2.10	2.05
19	3	614	LUT	C28-C29	-2.19	1.41	1.45
18	G	204	CLA	MG-NC	2.19	2.11	2.06
18	B	836	CLA	MG-NB	2.19	2.10	2.05
18	A	839	CLA	MG-NC	2.19	2.11	2.06
18	3	604	CLA	MG-NC	2.19	2.11	2.06
18	F	303	CLA	MG-NC	2.19	2.11	2.06
18	A	803	CLA	CHB-C1B	-2.18	1.34	1.39
18	4	609	CLA	MG-NB	2.18	2.10	2.05
18	A	837	CLA	C1B-NB	-2.18	1.35	1.37
18	B	814	CLA	C1B-NB	-2.18	1.35	1.37
18	1	610	CLA	CHB-C1B	-2.18	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	4	611	CLA	MG-NC	2.18	2.11	2.06
18	1	609	CLA	MG-NB	2.18	2.10	2.05
18	B	804	CLA	C1B-NB	-2.18	1.35	1.37
18	2	602	CLA	MG-NB	2.18	2.10	2.05
18	B	809	CLA	CHB-C1B	-2.18	1.34	1.39
18	2	604	CLA	MG-NB	2.18	2.10	2.05
18	A	837	CLA	MG-NB	2.18	2.10	2.05
18	4	601	CLA	C1B-NB	-2.18	1.35	1.37
18	B	805	CLA	MG-NB	2.18	2.10	2.05
18	B	814	CLA	MG-NB	2.18	2.10	2.05
18	G	203	CLA	CHB-C1B	-2.18	1.34	1.39
18	B	813	CLA	CHB-C1B	-2.18	1.34	1.39
18	A	804	CLA	MG-NB	2.18	2.10	2.05
18	B	826	CLA	MG-NB	2.18	2.10	2.05
18	L	303	CLA	CHB-C1B	-2.18	1.34	1.39
18	G	202	CLA	MG-NC	2.18	2.11	2.06
18	2	612	CLA	CHB-C1B	-2.17	1.34	1.39
18	A	806	CLA	C1B-NB	-2.17	1.35	1.37
18	F	301	CLA	CHB-C1B	-2.17	1.34	1.39
18	A	808	CLA	C1B-NB	-2.17	1.35	1.37
18	A	812	CLA	C1B-NB	-2.17	1.35	1.37
18	A	830	CLA	CHB-C1B	-2.17	1.34	1.39
18	A	805	CLA	MG-NB	2.17	2.10	2.05
18	A	835	CLA	CHB-C1B	-2.17	1.34	1.39
18	2	610	CLA	MG-NC	2.17	2.11	2.06
18	A	818	CLA	CHB-C1B	-2.17	1.34	1.39
18	A	816	CLA	MG-NC	2.17	2.11	2.06
18	B	807	CLA	MG-NC	2.17	2.11	2.06
18	3	606	CLA	MG-NC	2.17	2.11	2.06
18	2	611	CLA	MG-NC	2.17	2.11	2.06
18	B	837	CLA	MG-NC	2.17	2.11	2.06
18	A	830	CLA	MG-NB	2.17	2.10	2.05
18	2	609	CLA	CHB-C1B	-2.17	1.34	1.39
18	L	302	CLA	MG-NC	2.17	2.11	2.06
18	4	613	CLA	MG-NB	2.17	2.10	2.05
18	L	304	CLA	MG-NC	2.17	2.11	2.06
18	B	810	CLA	MG-NB	2.17	2.10	2.05
18	A	842	CLA	MG-NC	2.17	2.11	2.06
18	3	602	CLA	CHB-C1B	-2.17	1.34	1.39
18	B	808	CLA	MG-NC	2.16	2.11	2.06
18	B	832	CLA	CHB-C1B	-2.16	1.34	1.39
18	B	807	CLA	CHC-C1C	2.16	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	832	CLA	MG-NB	2.16	2.10	2.05
18	1	613	CLA	MG-NC	2.16	2.11	2.06
18	4	613	CLA	MG-NC	2.16	2.11	2.06
18	B	836	CLA	C1B-NB	-2.16	1.35	1.37
18	4	604	CLA	MG-NC	2.16	2.11	2.06
18	B	818	CLA	MG-NC	2.16	2.11	2.06
18	B	819	CLA	MG-NC	2.16	2.11	2.06
18	B	817	CLA	MG-NB	2.16	2.10	2.05
18	3	613	CLA	MG-NB	2.16	2.10	2.05
18	1	612	CLA	MG-NB	2.16	2.10	2.05
18	2	603	CLA	MG-NB	2.16	2.10	2.05
18	A	809	CLA	MG-NB	2.16	2.10	2.05
18	1	602	CLA	MG-NC	2.16	2.11	2.06
18	B	825	CLA	CHB-C1B	-2.16	1.34	1.39
18	H	201	CLA	MG-NC	2.16	2.11	2.06
18	A	827	CLA	MG-NB	2.16	2.10	2.05
18	1	603	CLA	C1B-NB	-2.16	1.35	1.37
18	3	617	CLA	C1B-NB	-2.16	1.35	1.37
18	B	839	CLA	CHC-C1C	2.15	1.42	1.38
18	2	609	CLA	MG-NB	2.15	2.10	2.05
18	2	613	CLA	MG-NC	2.15	2.11	2.06
18	3	602	CLA	MG-NC	2.15	2.11	2.06
18	B	815	CLA	MG-NC	2.15	2.11	2.06
18	3	613	CLA	MG-NC	2.15	2.11	2.06
18	A	838	CLA	C1B-NB	-2.15	1.35	1.37
18	4	602	CLA	MG-NC	2.15	2.11	2.06
18	B	819	CLA	CHB-C1B	-2.15	1.34	1.39
18	2	612	CLA	MG-NC	2.15	2.11	2.06
18	1	605	CLA	MG-NC	2.15	2.11	2.06
18	F	304	CLA	MG-NC	2.15	2.11	2.06
18	B	837	CLA	CHB-C1B	-2.15	1.34	1.39
18	3	611	CLA	MG-NC	2.15	2.11	2.06
18	A	813	CLA	MG-NB	2.15	2.10	2.05
18	A	833	CLA	MG-NC	2.15	2.11	2.06
18	F	304	CLA	C1B-NB	-2.15	1.35	1.37
18	1	604	CLA	MG-NC	2.15	2.11	2.06
18	B	830	CLA	C1B-NB	-2.15	1.35	1.37
18	A	833	CLA	C1B-NB	-2.14	1.35	1.37
18	2	612	CLA	MG-NB	2.14	2.10	2.05
18	A	826	CLA	MG-NB	2.14	2.10	2.05
18	A	828	CLA	MG-NC	2.14	2.11	2.06
18	B	827	CLA	C1B-NB	-2.14	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	826	CLA	MG-NC	2.14	2.11	2.06
18	A	829	CLA	MG-NB	2.14	2.10	2.05
18	B	828	CLA	C1B-NB	-2.14	1.35	1.37
18	B	808	CLA	C1B-NB	-2.14	1.35	1.37
18	A	802	CLA	CHB-C1B	-2.14	1.34	1.39
18	A	801	CLA	MG-NB	2.14	2.10	2.05
18	F	301	CLA	MG-NB	2.14	2.10	2.05
18	B	809	CLA	C1B-NB	-2.14	1.35	1.37
18	A	807	CLA	MG-NB	2.14	2.10	2.05
18	A	815	CLA	C1B-NB	-2.14	1.35	1.37
18	B	810	CLA	C1B-NB	-2.14	1.35	1.37
18	3	602	CLA	MG-NB	2.14	2.10	2.05
18	A	836	CLA	CHB-C1B	-2.14	1.34	1.39
18	3	605	CLA	MG-NC	2.14	2.11	2.06
18	B	835	CLA	MG-NC	2.14	2.11	2.06
18	B	827	CLA	MG-NC	2.14	2.11	2.06
18	1	610	CLA	MG-NC	2.14	2.11	2.06
18	B	830	CLA	MG-NB	2.14	2.10	2.05
18	A	817	CLA	MG-NC	2.14	2.11	2.06
18	K	203	CLA	MG-NC	2.14	2.11	2.06
18	A	820	CLA	MG-NC	2.13	2.11	2.06
18	A	837	CLA	MG-NC	2.13	2.11	2.06
18	B	823	CLA	MG-NC	2.13	2.11	2.06
18	2	608	CLA	C1B-NB	-2.13	1.35	1.37
18	1	607	CLA	MG-NC	2.13	2.11	2.06
18	A	803	CLA	MG-NC	2.13	2.11	2.06
18	A	830	CLA	MG-NC	2.13	2.11	2.06
18	B	824	CLA	C1B-NB	-2.13	1.35	1.37
18	B	805	CLA	MG-NC	2.13	2.11	2.06
18	B	839	CLA	MG-NC	2.13	2.11	2.06
18	A	804	CLA	MG-NC	2.13	2.11	2.06
18	F	301	CLA	MG-NC	2.13	2.11	2.06
18	F	304	CLA	MG-NB	2.13	2.10	2.05
18	B	812	CLA	MG-NB	2.13	2.10	2.05
18	A	825	CLA	C1B-NB	-2.13	1.35	1.37
18	B	802	CLA	C1B-NB	-2.13	1.35	1.37
18	4	612	CLA	MG-NB	2.13	2.10	2.05
18	B	815	CLA	MG-NB	2.13	2.10	2.05
18	A	827	CLA	MG-NC	2.13	2.11	2.06
18	1	608	CLA	MG-NC	2.13	2.11	2.06
18	1	611	CLA	MG-NC	2.13	2.11	2.06
18	2	604	CLA	MG-NC	2.13	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	819	CLA	C1B-NB	-2.13	1.35	1.37
18	A	807	CLA	MG-NC	2.13	2.11	2.06
18	A	808	CLA	MG-NC	2.13	2.11	2.06
18	A	821	CLA	MG-NC	2.13	2.11	2.06
18	B	813	CLA	MG-NC	2.13	2.11	2.06
18	A	820	CLA	MG-NB	2.13	2.10	2.05
18	B	818	CLA	MG-NB	2.12	2.10	2.05
18	A	807	CLA	C1B-NB	-2.12	1.35	1.37
18	4	614	CLA	MG-NB	2.12	2.10	2.05
18	3	617	CLA	MG-NB	2.12	2.10	2.05
18	B	825	CLA	MG-NC	2.12	2.11	2.06
18	B	806	CLA	MG-NB	2.12	2.10	2.05
18	B	839	CLA	C1B-NB	-2.12	1.35	1.37
18	A	801	CLA	MG-NC	2.12	2.11	2.06
18	B	830	CLA	MG-NC	2.12	2.11	2.06
18	A	831	CLA	MG-NB	2.12	2.10	2.05
18	A	816	CLA	C1B-NB	-2.12	1.35	1.37
18	B	831	CLA	C1B-NB	-2.12	1.35	1.37
18	4	602	CLA	C1B-NB	-2.12	1.35	1.37
18	A	841	CLA	MG-NC	2.12	2.11	2.06
18	A	835	CLA	C1B-NB	-2.12	1.35	1.37
18	A	818	CLA	MG-NB	2.12	2.10	2.05
18	A	822	CLA	MG-NC	2.12	2.11	2.06
18	A	815	CLA	MG-NB	2.12	2.10	2.05
18	A	838	CLA	MG-NC	2.11	2.11	2.06
18	A	824	CLA	MG-NB	2.11	2.10	2.05
18	G	203	CLA	MG-NB	2.11	2.10	2.05
18	A	824	CLA	C1B-NB	-2.11	1.35	1.37
18	A	836	CLA	MG-NC	2.11	2.11	2.06
18	G	203	CLA	MG-NC	2.11	2.11	2.06
18	H	201	CLA	MG-NB	2.11	2.10	2.05
18	4	608	CLA	C1B-NB	-2.11	1.35	1.37
18	A	827	CLA	C1B-NB	-2.11	1.35	1.37
17	2	607	CHL	C3B-CAB	-2.11	1.43	1.47
18	2	602	CLA	MG-NC	2.11	2.11	2.06
18	B	840	CLA	MG-NC	2.11	2.11	2.06
18	A	824	CLA	MG-NC	2.11	2.11	2.06
18	B	814	CLA	MG-NC	2.11	2.11	2.06
17	4	605	CHL	C3B-CAB	-2.11	1.43	1.47
18	3	609	CLA	MG-NC	2.11	2.11	2.06
18	A	811	CLA	MG-NC	2.11	2.11	2.06
18	A	817	CLA	C1B-NB	-2.11	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	829	CLA	MG-NC	2.11	2.11	2.06
18	A	813	CLA	MG-NC	2.11	2.11	2.06
18	A	831	CLA	C1B-NB	-2.11	1.35	1.37
18	A	833	CLA	CHC-C1C	2.11	1.42	1.38
18	1	612	CLA	MG-NC	2.11	2.11	2.06
18	B	809	CLA	MG-NC	2.11	2.11	2.06
18	B	822	CLA	C1B-NB	-2.11	1.35	1.37
18	4	601	CLA	MG-NC	2.11	2.11	2.06
18	A	829	CLA	MG-NC	2.11	2.11	2.06
18	3	608	CLA	MG-NC	2.10	2.11	2.06
18	A	826	CLA	MG-NC	2.10	2.11	2.06
18	B	808	CLA	MG-NB	2.10	2.10	2.05
18	A	821	CLA	MG-NB	2.10	2.10	2.05
18	A	839	CLA	C1B-NB	-2.10	1.35	1.37
18	A	843	CLA	CHB-C1B	-2.10	1.34	1.39
18	A	809	CLA	MG-NC	2.10	2.11	2.06
18	A	814	CLA	MG-NC	2.10	2.11	2.06
18	A	832	CLA	MG-NC	2.10	2.11	2.06
18	L	303	CLA	C1B-NB	-2.10	1.35	1.37
18	B	810	CLA	C3B-C2B	-2.10	1.36	1.44
18	A	805	CLA	MG-NC	2.10	2.11	2.06
18	B	817	CLA	C1B-NB	-2.10	1.35	1.37
18	B	804	CLA	MG-NC	2.10	2.11	2.06
18	3	617	CLA	MG-NC	2.10	2.11	2.06
18	A	801	CLA	CHB-C1B	-2.10	1.34	1.39
18	3	613	CLA	C1B-NB	-2.10	1.35	1.37
18	1	614	CLA	MG-NC	2.10	2.11	2.06
18	4	612	CLA	MG-NC	2.10	2.11	2.06
18	A	835	CLA	MG-NC	2.10	2.11	2.06
18	B	824	CLA	MG-NB	2.10	2.10	2.05
18	A	812	CLA	MG-NC	2.10	2.11	2.06
17	4	607	CHL	C3B-CAB	-2.10	1.43	1.47
18	B	825	CLA	MG-NB	2.10	2.09	2.05
18	B	819	CLA	MG-NB	2.10	2.09	2.05
18	2	603	CLA	MG-NC	2.10	2.11	2.06
18	1	614	CLA	C1B-NB	-2.10	1.35	1.37
18	B	805	CLA	C1B-NB	-2.10	1.35	1.37
18	2	608	CLA	MG-NC	2.10	2.11	2.06
18	A	819	CLA	C1B-NB	-2.10	1.35	1.37
18	4	614	CLA	C1B-NB	-2.09	1.35	1.37
18	A	812	CLA	MG-NB	2.09	2.09	2.05
18	A	819	CLA	MG-NC	2.09	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	822	CLA	C1B-NB	-2.09	1.35	1.37
18	B	801	CLA	MG-NC	2.09	2.11	2.06
18	4	603	CLA	CHC-C1C	2.09	1.42	1.38
18	4	601	CLA	MG-NB	2.09	2.09	2.05
18	A	831	CLA	MG-NC	2.09	2.11	2.06
18	B	812	CLA	C1B-NB	-2.09	1.35	1.37
18	A	806	CLA	MG-NC	2.09	2.11	2.06
18	1	609	CLA	MG-NC	2.09	2.11	2.06
18	A	814	CLA	MG-NB	2.09	2.09	2.05
17	4	615	CHL	C2C-C3C	2.09	1.38	1.36
18	B	802	CLA	CHB-C1B	-2.09	1.34	1.39
17	2	605	CHL	CAC-C3C	2.09	1.54	1.50
18	A	834	CLA	MG-NB	2.08	2.09	2.05
17	4	606	CHL	C3B-CAB	-2.08	1.43	1.47
18	A	815	CLA	MG-NC	2.08	2.11	2.06
18	L	303	CLA	MG-NB	2.08	2.09	2.05
18	1	607	CLA	C1B-NB	-2.08	1.35	1.37
18	B	817	CLA	MG-NC	2.08	2.11	2.06
17	2	605	CHL	C3B-CAB	-2.08	1.43	1.47
18	A	832	CLA	C1B-NB	-2.08	1.35	1.37
18	2	603	CLA	C1B-NB	-2.08	1.35	1.37
18	B	824	CLA	MG-NC	2.08	2.11	2.06
18	B	813	CLA	C1B-NB	-2.07	1.35	1.37
18	4	608	CLA	MG-NC	2.07	2.11	2.06
18	B	810	CLA	MG-NC	2.07	2.11	2.06
18	A	840	CLA	MG-NC	2.07	2.11	2.06
18	B	809	CLA	MG-NB	2.07	2.09	2.05
18	1	611	CLA	C1B-NB	-2.07	1.35	1.37
18	B	813	CLA	MG-NB	2.07	2.09	2.05
18	B	833	CLA	C1B-NB	-2.07	1.35	1.37
18	A	834	CLA	MG-NC	2.07	2.11	2.06
18	L	303	CLA	MG-NC	2.07	2.11	2.06
18	A	804	CLA	C1B-NB	-2.07	1.35	1.37
18	A	809	CLA	C1B-NB	-2.07	1.35	1.37
18	A	801	CLA	C1B-NB	-2.07	1.35	1.37
18	B	806	CLA	MG-NC	2.07	2.11	2.06
18	A	818	CLA	MG-NC	2.07	2.11	2.06
18	B	833	CLA	MG-NC	2.07	2.11	2.06
18	A	841	CLA	C1B-NB	-2.07	1.35	1.37
18	B	816	CLA	MG-NC	2.07	2.11	2.06
18	G	202	CLA	C1B-NB	-2.07	1.35	1.37
18	B	821	CLA	MG-NC	2.07	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	B	833	CLA	MG-NB	2.07	2.09	2.05
18	2	612	CLA	C1B-NB	-2.07	1.35	1.37
18	4	611	CLA	C1B-NB	-2.07	1.35	1.37
18	3	608	CLA	C1B-NB	-2.06	1.35	1.37
18	4	602	CLA	MG-NB	2.06	2.09	2.05
18	B	811	CLA	MG-NC	2.06	2.11	2.06
18	B	802	CLA	MG-NB	2.06	2.09	2.05
17	1	601	CHL	C3B-CAB	-2.06	1.43	1.47
17	1	606	CHL	C3B-CAB	-2.06	1.43	1.47
18	L	302	CLA	C1B-NB	-2.06	1.35	1.37
18	B	802	CLA	MG-NC	2.06	2.11	2.06
18	3	604	CLA	C1B-NB	-2.06	1.35	1.37
18	A	836	CLA	C1B-NB	-2.06	1.35	1.37
18	B	822	CLA	MG-NC	2.05	2.11	2.06
18	B	826	CLA	C1B-NB	-2.05	1.35	1.37
18	B	839	CLA	MG-NB	2.05	2.09	2.05
18	K	201	CLA	CAA-C2A	2.05	1.57	1.53
18	2	604	CLA	C1B-NB	-2.05	1.35	1.37
18	2	611	CLA	C1B-NB	-2.05	1.35	1.37
18	A	822	CLA	MG-NB	2.05	2.09	2.05
18	B	820	CLA	MG-NC	2.05	2.11	2.06
18	3	612	CLA	CAA-C2A	2.05	1.57	1.53
18	G	203	CLA	C1B-NB	-2.05	1.35	1.37
18	H	201	CLA	C1B-NB	-2.05	1.35	1.37
18	A	802	CLA	C3D-C4D	-2.05	1.39	1.44
17	2	601	CHL	C3B-CAB	-2.05	1.43	1.47
18	A	830	CLA	C1B-NB	-2.05	1.35	1.37
18	B	828	CLA	MG-NC	2.04	2.11	2.06
18	B	801	CLA	C1B-NB	-2.04	1.35	1.37
17	2	606	CHL	C3B-CAB	-2.04	1.43	1.47
18	1	612	CLA	C1B-NB	-2.04	1.35	1.37
18	2	609	CLA	C1B-NB	-2.04	1.35	1.37
18	B	803	CLA	MG-NC	2.04	2.11	2.06
18	1	603	CLA	MG-NC	2.04	2.11	2.06
18	A	810	CLA	MG-NC	2.04	2.11	2.06
18	B	831	CLA	CAA-C2A	2.04	1.57	1.54
18	1	613	CLA	C1B-NB	-2.04	1.35	1.37
18	L	304	CLA	C1B-NB	-2.04	1.35	1.37
18	B	821	CLA	C1B-NB	-2.04	1.35	1.37
18	B	840	CLA	C1B-NB	-2.04	1.35	1.37
18	1	614	CLA	MG-NB	2.03	2.09	2.05
18	2	609	CLA	MG-NC	2.03	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	835	CLA	MG-NB	2.03	2.09	2.05
18	F	304	CLA	CAA-C2A	2.03	1.57	1.53
18	4	612	CLA	C1B-NB	-2.03	1.35	1.37
18	A	802	CLA	MG-NC	2.03	2.11	2.06
18	B	829	CLA	MG-NB	2.03	2.09	2.05
18	A	823	CLA	CAA-C2A	2.02	1.57	1.53
18	B	836	CLA	MG-NC	2.02	2.11	2.06
18	3	607	CLA	C1B-NB	-2.02	1.35	1.37
18	B	822	CLA	CHD-C1D	2.02	1.42	1.38
18	1	602	CLA	C1B-NB	-2.02	1.35	1.37
18	A	806	CLA	MG-NB	2.02	2.09	2.05
18	B	834	CLA	C1B-NB	-2.02	1.35	1.37
18	4	609	CLA	C1B-NB	-2.02	1.35	1.37
18	A	810	CLA	MG-NB	2.02	2.09	2.05
18	2	602	CLA	C1B-NB	-2.02	1.35	1.37
18	4	609	CLA	MG-NC	2.02	2.11	2.06
18	B	822	CLA	MG-NB	2.01	2.09	2.05
17	2	606	CHL	O1D-CGD	2.01	1.26	1.21
18	4	613	CLA	C1B-NB	-2.01	1.35	1.37
18	2	613	CLA	C1B-NB	-2.01	1.35	1.37
17	3	616	CHL	C3B-CAB	-2.01	1.43	1.47
18	A	811	CLA	C1B-NB	-2.01	1.35	1.37
18	3	602	CLA	C1B-NB	-2.01	1.35	1.37
18	3	611	CLA	C1B-NB	-2.01	1.35	1.37
18	B	815	CLA	C1B-NB	-2.00	1.35	1.37
18	B	820	CLA	MG-NB	2.00	2.09	2.05
18	B	838	CLA	C1B-NB	-2.00	1.35	1.37

All (1618) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	601	CHL	C1B-CHB-C4A	13.32	129.55	121.39
17	3	616	CHL	C1B-CHB-C4A	13.07	129.40	121.39
17	2	606	CHL	C1B-CHB-C4A	12.87	129.27	121.39
17	4	607	CHL	C1B-CHB-C4A	12.84	129.26	121.39
17	4	615	CHL	C1B-CHB-C4A	12.81	129.24	121.39
17	2	607	CHL	C1B-CHB-C4A	12.81	129.24	121.39
17	2	601	CHL	C1B-CHB-C4A	12.64	129.13	121.39
17	2	605	CHL	C1B-CHB-C4A	12.63	129.13	121.39
17	2	614	CHL	C1B-CHB-C4A	12.61	129.12	121.39
17	4	606	CHL	C1B-CHB-C4A	12.61	129.12	121.39
17	1	606	CHL	C1B-CHB-C4A	12.58	129.10	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CHL	C1B-CHB-C4A	12.55	129.08	121.39
18	B	802	CLA	C4A-NA-C1A	11.39	111.83	106.71
18	A	837	CLA	C4A-NA-C1A	11.20	111.74	106.71
18	B	805	CLA	C4A-NA-C1A	11.11	111.70	106.71
18	2	612	CLA	C4A-NA-C1A	11.08	111.69	106.71
18	A	813	CLA	C4A-NA-C1A	11.06	111.68	106.71
18	A	827	CLA	C4A-NA-C1A	11.03	111.67	106.71
18	B	804	CLA	C4A-NA-C1A	10.91	111.61	106.71
18	B	831	CLA	C4A-NA-C1A	10.86	111.59	106.71
18	A	807	CLA	C4A-NA-C1A	10.83	111.57	106.71
18	B	812	CLA	C4A-NA-C1A	10.75	111.54	106.71
18	1	603	CLA	C4A-NA-C1A	10.71	111.52	106.71
18	K	203	CLA	C4A-NA-C1A	10.71	111.52	106.71
18	A	806	CLA	C4A-NA-C1A	10.70	111.52	106.71
18	4	611	CLA	C4A-NA-C1A	10.64	111.49	106.71
18	F	304	CLA	C4A-NA-C1A	10.64	111.49	106.71
18	B	837	CLA	C4A-NA-C1A	10.60	111.47	106.71
18	L	304	CLA	C4A-NA-C1A	10.60	111.47	106.71
18	1	611	CLA	C4A-NA-C1A	10.57	111.46	106.71
18	A	802	CLA	C4A-NA-C1A	10.57	111.46	106.71
18	B	807	CLA	C4A-NA-C1A	10.56	111.45	106.71
18	A	834	CLA	C4A-NA-C1A	10.56	111.45	106.71
18	A	805	CLA	C4A-NA-C1A	10.54	111.45	106.71
18	B	814	CLA	C4A-NA-C1A	10.54	111.44	106.71
18	4	608	CLA	C4A-NA-C1A	10.53	111.44	106.71
18	B	834	CLA	C4A-NA-C1A	10.53	111.44	106.71
18	A	804	CLA	C4A-NA-C1A	10.53	111.44	106.71
18	A	816	CLA	C4A-NA-C1A	10.52	111.44	106.71
18	B	839	CLA	C4A-NA-C1A	10.51	111.43	106.71
18	2	611	CLA	C4A-NA-C1A	10.51	111.43	106.71
18	A	836	CLA	C4A-NA-C1A	10.50	111.42	106.71
18	A	833	CLA	C4A-NA-C1A	10.48	111.42	106.71
18	A	801	CLA	C4A-NA-C1A	10.47	111.42	106.71
18	B	835	CLA	C4A-NA-C1A	10.42	111.39	106.71
18	A	842	CLA	C4A-NA-C1A	10.40	111.38	106.71
18	1	604	CLA	C4A-NA-C1A	10.38	111.37	106.71
18	A	840	CLA	C4A-NA-C1A	10.35	111.36	106.71
18	B	819	CLA	C4A-NA-C1A	10.33	111.35	106.71
18	3	603	CLA	C4A-NA-C1A	10.32	111.34	106.71
18	A	820	CLA	C4A-NA-C1A	10.32	111.34	106.71
18	3	606	CLA	C4A-NA-C1A	10.29	111.33	106.71
18	3	605	CLA	C4A-NA-C1A	10.29	111.33	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	203	CLA	C4A-NA-C1A	10.27	111.32	106.71
18	4	603	CLA	C4A-NA-C1A	10.27	111.32	106.71
18	3	607	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	B	810	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	B	829	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	A	828	CLA	C4A-NA-C1A	10.26	111.32	106.71
18	1	612	CLA	C4A-NA-C1A	10.25	111.32	106.71
18	A	811	CLA	C4A-NA-C1A	10.23	111.31	106.71
18	L	302	CLA	C4A-NA-C1A	10.21	111.30	106.71
18	A	841	CLA	C4A-NA-C1A	10.21	111.30	106.71
18	B	815	CLA	C4A-NA-C1A	10.20	111.29	106.71
18	G	202	CLA	C4A-NA-C1A	10.20	111.29	106.71
18	1	613	CLA	C4A-NA-C1A	10.19	111.29	106.71
18	3	610	CLA	C4A-NA-C1A	10.19	111.29	106.71
18	B	817	CLA	C4A-NA-C1A	10.17	111.28	106.71
18	B	813	CLA	C4A-NA-C1A	10.15	111.27	106.71
18	B	826	CLA	C4A-NA-C1A	10.13	111.26	106.71
18	A	808	CLA	C4A-NA-C1A	10.12	111.25	106.71
18	A	809	CLA	C4A-NA-C1A	10.11	111.25	106.71
18	2	609	CLA	C4A-NA-C1A	10.11	111.25	106.71
18	A	814	CLA	C4A-NA-C1A	10.10	111.25	106.71
18	1	607	CLA	C4A-NA-C1A	10.07	111.23	106.71
18	1	610	CLA	C4A-NA-C1A	10.06	111.23	106.71
18	A	812	CLA	C4A-NA-C1A	10.05	111.22	106.71
18	2	613	CLA	C4A-NA-C1A	10.04	111.22	106.71
18	1	614	CLA	C4A-NA-C1A	10.04	111.22	106.71
18	4	612	CLA	C4A-NA-C1A	10.03	111.21	106.71
18	4	613	CLA	C4A-NA-C1A	10.02	111.21	106.71
18	3	617	CLA	C4A-NA-C1A	10.00	111.20	106.71
18	A	829	CLA	C4A-NA-C1A	9.99	111.20	106.71
18	A	839	CLA	C4A-NA-C1A	9.98	111.19	106.71
18	2	603	CLA	C4A-NA-C1A	9.97	111.19	106.71
18	F	303	CLA	C4A-NA-C1A	9.97	111.19	106.71
18	1	605	CLA	C4A-NA-C1A	9.96	111.19	106.71
18	B	828	CLA	C4A-NA-C1A	9.95	111.18	106.71
18	2	604	CLA	C4A-NA-C1A	9.94	111.18	106.71
18	3	613	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	J	102	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	3	602	CLA	C4A-NA-C1A	9.94	111.17	106.71
18	B	823	CLA	C4A-NA-C1A	9.93	111.17	106.71
18	3	611	CLA	C4A-NA-C1A	9.93	111.17	106.71
18	4	601	CLA	C4A-NA-C1A	9.92	111.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	843	CLA	C4A-NA-C1A	9.91	111.16	106.71
18	B	840	CLA	C4A-NA-C1A	9.90	111.16	106.71
18	3	608	CLA	C4A-NA-C1A	9.89	111.15	106.71
18	B	838	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	B	827	CLA	C4A-NA-C1A	9.88	111.15	106.71
18	A	838	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	A	831	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	K	201	CLA	C4A-NA-C1A	9.87	111.14	106.71
18	A	835	CLA	C4A-NA-C1A	9.86	111.14	106.71
18	A	823	CLA	C4A-NA-C1A	9.86	111.14	106.71
18	4	604	CLA	C4A-NA-C1A	9.84	111.13	106.71
18	B	811	CLA	C4A-NA-C1A	9.82	111.12	106.71
18	G	204	CLA	C4A-NA-C1A	9.82	111.12	106.71
18	1	602	CLA	C4A-NA-C1A	9.81	111.12	106.71
18	A	830	CLA	C4A-NA-C1A	9.77	111.10	106.71
18	A	803	CLA	C4A-NA-C1A	9.76	111.10	106.71
18	B	833	CLA	C4A-NA-C1A	9.76	111.09	106.71
18	1	608	CLA	C4A-NA-C1A	9.76	111.09	106.71
18	4	609	CLA	C4A-NA-C1A	9.74	111.09	106.71
18	B	825	CLA	C4A-NA-C1A	9.74	111.08	106.71
18	B	830	CLA	C4A-NA-C1A	9.73	111.08	106.71
18	A	832	CLA	C4A-NA-C1A	9.72	111.08	106.71
18	4	614	CLA	C4A-NA-C1A	9.71	111.07	106.71
18	L	303	CLA	C4A-NA-C1A	9.71	111.07	106.71
18	3	604	CLA	C4A-NA-C1A	9.70	111.07	106.71
18	A	821	CLA	C4A-NA-C1A	9.70	111.07	106.71
18	B	836	CLA	C4A-NA-C1A	9.64	111.04	106.71
18	A	826	CLA	C4A-NA-C1A	9.62	111.03	106.71
18	1	609	CLA	C4A-NA-C1A	9.60	111.02	106.71
18	A	819	CLA	C4A-NA-C1A	9.60	111.02	106.71
18	B	818	CLA	C4A-NA-C1A	9.59	111.02	106.71
18	A	818	CLA	C4A-NA-C1A	9.58	111.01	106.71
18	4	602	CLA	C4A-NA-C1A	9.54	111.00	106.71
18	B	801	CLA	C4A-NA-C1A	9.52	110.98	106.71
18	B	806	CLA	C4A-NA-C1A	9.52	110.98	106.71
18	B	808	CLA	C4A-NA-C1A	9.51	110.98	106.71
18	B	821	CLA	C4A-NA-C1A	9.49	110.97	106.71
18	A	817	CLA	C4A-NA-C1A	9.48	110.97	106.71
18	A	815	CLA	C4A-NA-C1A	9.48	110.97	106.71
18	2	610	CLA	C4A-NA-C1A	9.47	110.97	106.71
18	F	301	CLA	C4A-NA-C1A	9.46	110.96	106.71
18	4	610	CLA	C4A-NA-C1A	9.46	110.96	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	H	201	CLA	C4A-NA-C1A	9.44	110.95	106.71
18	2	602	CLA	C4A-NA-C1A	9.39	110.93	106.71
18	2	608	CLA	C4A-NA-C1A	9.37	110.92	106.71
18	A	825	CLA	C4A-NA-C1A	9.28	110.88	106.71
18	B	803	CLA	C4A-NA-C1A	9.27	110.87	106.71
18	B	820	CLA	C4A-NA-C1A	9.26	110.87	106.71
18	K	202	CLA	C4A-NA-C1A	9.25	110.86	106.71
18	A	822	CLA	C4A-NA-C1A	9.20	110.84	106.71
18	B	832	CLA	C4A-NA-C1A	9.18	110.83	106.71
18	B	809	CLA	C4A-NA-C1A	9.14	110.81	106.71
18	3	609	CLA	C4A-NA-C1A	9.09	110.79	106.71
18	A	824	CLA	C4A-NA-C1A	9.03	110.77	106.71
18	3	612	CLA	C4A-NA-C1A	9.01	110.76	106.71
18	A	810	CLA	C4A-NA-C1A	9.00	110.75	106.71
18	B	824	CLA	C4A-NA-C1A	8.97	110.74	106.71
18	B	816	CLA	C4A-NA-C1A	8.75	110.64	106.71
18	A	854	CLA	C4A-NA-C1A	8.72	110.63	106.71
18	B	822	CLA	C4A-NA-C1A	8.19	110.39	106.71
18	B	810	CLA	CAB-C3B-C4B	7.88	137.37	125.37
17	4	606	CHL	O2D-CGD-CBD	6.07	118.68	111.00
17	4	605	CHL	O2D-CGD-CBD	6.05	118.66	111.00
17	4	607	CHL	O2D-CGD-CBD	6.01	118.61	111.00
17	2	601	CHL	O2D-CGD-CBD	5.94	118.53	111.00
17	2	607	CHL	O2D-CGD-CBD	5.73	118.26	111.00
17	3	616	CHL	O2D-CGD-CBD	5.69	118.21	111.00
17	2	614	CHL	O2D-CGD-CBD	5.52	117.99	111.00
17	2	605	CHL	O2D-CGD-CBD	5.40	117.83	111.00
17	2	606	CHL	O2D-CGD-CBD	5.39	117.82	111.00
19	3	614	LUT	C15-C35-C34	5.39	134.51	123.47
17	1	606	CHL	CAA-C2A-C3A	-5.36	103.58	116.10
17	2	607	CHL	C4D-CHA-CBD	-4.81	103.93	108.89
17	3	616	CHL	C3D-C4D-CHA	4.78	115.81	108.54
18	B	806	CLA	O2D-CGD-CBD	4.75	119.71	111.27
17	3	616	CHL	CBC-CAC-C3C	-4.66	106.06	112.88
18	A	831	CLA	O2D-CGD-CBD	4.64	119.52	111.27
17	4	615	CHL	C3D-C4D-CHA	4.62	115.57	108.54
17	2	607	CHL	C3D-C4D-CHA	4.61	115.56	108.54
17	2	601	CHL	C4D-CHA-CBD	-4.60	104.15	108.89
17	2	614	CHL	C3D-C4D-CHA	4.60	115.53	108.54
18	B	807	CLA	O2D-CGD-CBD	4.59	119.42	111.27
18	B	837	CLA	O2D-CGD-CBD	4.59	119.42	111.27
17	1	606	CHL	C3D-C4D-CHA	4.58	115.50	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	3	616	CHL	C4D-CHA-CBD	-4.58	104.17	108.89
18	A	816	CLA	O2D-CGD-CBD	4.56	119.37	111.27
17	4	605	CHL	C3D-C4D-CHA	4.55	115.46	108.54
17	1	601	CHL	C3D-C4D-CHA	4.55	115.45	108.54
17	2	605	CHL	C4D-CHA-CBD	-4.53	104.22	108.89
17	4	606	CHL	C3D-C4D-CHA	4.53	115.42	108.54
18	B	812	CLA	O2D-CGD-CBD	4.52	119.30	111.27
17	2	601	CHL	C3D-C4D-CHA	4.50	115.38	108.54
17	4	607	CHL	C3D-C4D-CHA	4.49	115.37	108.54
17	2	606	CHL	C3D-C4D-CHA	4.49	115.37	108.54
18	B	832	CLA	O2D-CGD-CBD	4.48	119.23	111.27
18	B	819	CLA	O2D-CGD-CBD	4.46	119.19	111.27
18	B	816	CLA	O2D-CGD-CBD	4.45	119.18	111.27
19	3	614	LUT	C39-C29-C30	-4.44	116.71	122.92
17	2	605	CHL	C3D-C4D-CHA	4.43	115.27	108.54
17	4	605	CHL	C4D-CHA-CBD	-4.38	104.37	108.89
18	B	809	CLA	O2D-CGD-CBD	4.38	119.06	111.27
18	B	804	CLA	O2D-CGD-CBD	4.38	119.05	111.27
18	B	821	CLA	O2D-CGD-CBD	4.38	119.05	111.27
17	4	607	CHL	C4D-CHA-CBD	-4.38	104.38	108.89
18	B	835	CLA	O2D-CGD-CBD	4.36	119.01	111.27
18	B	827	CLA	O2D-CGD-CBD	4.36	119.01	111.27
18	A	827	CLA	O2D-CGD-CBD	4.34	118.98	111.27
18	A	805	CLA	O2D-CGD-CBD	4.33	118.96	111.27
18	B	839	CLA	O2D-CGD-CBD	4.31	118.93	111.27
18	1	613	CLA	O2D-CGD-CBD	4.31	118.92	111.27
18	A	804	CLA	O2D-CGD-CBD	4.30	118.91	111.27
18	A	839	CLA	O2D-CGD-CBD	4.30	118.91	111.27
18	A	854	CLA	O2D-CGD-CBD	4.29	118.90	111.27
18	A	806	CLA	O2D-CGD-CBD	4.29	118.90	111.27
18	B	801	CLA	O2D-CGD-CBD	4.29	118.89	111.27
18	A	803	CLA	O2D-CGD-CBD	4.28	118.88	111.27
18	A	837	CLA	O2D-CGD-CBD	4.28	118.87	111.27
17	2	614	CHL	CAA-C2A-C3A	-4.28	103.58	114.26
18	A	820	CLA	O2D-CGD-CBD	4.27	118.86	111.27
18	B	815	CLA	O2D-CGD-CBD	4.27	118.85	111.27
18	4	610	CLA	O2D-CGD-CBD	4.27	118.85	111.27
18	A	818	CLA	O2D-CGD-CBD	4.26	118.84	111.27
17	4	607	CHL	CBC-CAC-C3C	-4.26	106.65	112.88
17	1	606	CHL	C4D-CHA-CBD	-4.23	104.53	108.89
18	B	826	CLA	O2D-CGD-CBD	4.22	118.76	111.27
18	A	813	CLA	O2D-CGD-CBD	4.22	118.76	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	830	CLA	O2D-CGD-CBD	4.22	118.76	111.27
18	B	840	CLA	O2D-CGD-CBD	4.21	118.75	111.27
17	1	601	CHL	C4D-CHA-CBD	-4.20	104.56	108.89
18	B	823	CLA	O2D-CGD-CBD	4.20	118.74	111.27
18	B	808	CLA	O2D-CGD-CBD	4.20	118.73	111.27
18	A	825	CLA	O2D-CGD-CBD	4.19	118.72	111.27
17	4	615	CHL	C4D-CHA-CBD	-4.19	104.58	108.89
18	B	814	CLA	O2D-CGD-CBD	4.18	118.70	111.27
18	A	838	CLA	O2D-CGD-CBD	4.18	118.70	111.27
17	4	615	CHL	CAA-C2A-C3A	-4.18	103.81	114.26
18	A	815	CLA	O2D-CGD-CBD	4.18	118.69	111.27
18	1	608	CLA	O2D-CGD-CBD	4.18	118.69	111.27
19	4	616	LUT	C15-C35-C34	4.18	132.03	123.47
18	B	810	CLA	C3B-C4B-NB	-4.17	107.44	110.23
19	1	619	LUT	C35-C15-C14	4.17	132.02	123.47
18	A	829	CLA	O2D-CGD-CBD	4.17	118.68	111.27
18	A	841	CLA	O2D-CGD-CBD	4.16	118.67	111.27
18	4	609	CLA	O2D-CGD-CBD	4.16	118.66	111.27
17	4	606	CHL	C4D-CHA-CBD	-4.16	104.60	108.89
17	2	605	CHL	CAA-C2A-C3A	-4.15	103.88	114.26
18	A	826	CLA	O2D-CGD-CBD	4.15	118.64	111.27
18	B	828	CLA	O2D-CGD-CBD	4.15	118.64	111.27
18	A	809	CLA	O2D-CGD-CBD	4.13	118.61	111.27
18	A	823	CLA	O2D-CGD-CBD	4.12	118.60	111.27
18	G	202	CLA	O2D-CGD-CBD	4.12	118.59	111.27
17	2	614	CHL	C4D-CHA-CBD	-4.12	104.64	108.89
18	A	830	CLA	O2D-CGD-CBD	4.12	118.59	111.27
18	4	601	CLA	O2D-CGD-CBD	4.12	118.59	111.27
18	A	833	CLA	O2D-CGD-CBD	4.11	118.58	111.27
18	1	609	CLA	O2D-CGD-CBD	4.11	118.58	111.27
18	B	825	CLA	O2D-CGD-CBD	4.11	118.57	111.27
18	F	301	CLA	O2D-CGD-CBD	4.11	118.57	111.27
17	2	606	CHL	CAA-C2A-C3A	-4.10	104.00	114.26
18	B	833	CLA	O2D-CGD-CBD	4.10	118.56	111.27
18	3	605	CLA	O2D-CGD-CBD	4.10	118.55	111.27
19	1	619	LUT	C19-C9-C10	-4.08	117.20	122.92
18	A	819	CLA	O2D-CGD-CBD	4.08	118.52	111.27
18	1	604	CLA	O2D-CGD-CBD	4.08	118.51	111.27
18	B	803	CLA	O2D-CGD-CBD	4.07	118.51	111.27
17	2	606	CHL	C4D-CHA-CBD	-4.07	104.69	108.89
18	B	811	CLA	O2D-CGD-CBD	4.07	118.50	111.27
18	3	608	CLA	O2D-CGD-CBD	4.07	118.50	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	303	CLA	O2D-CGD-CBD	4.07	118.49	111.27
18	4	612	CLA	O2D-CGD-CBD	4.06	118.48	111.27
18	1	605	CLA	O2D-CGD-CBD	4.05	118.47	111.27
18	G	204	CLA	O2D-CGD-CBD	4.05	118.47	111.27
18	4	608	CLA	O2D-CGD-CBD	4.05	118.46	111.27
18	3	602	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	3	617	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	J	102	CLA	O2D-CGD-CBD	4.03	118.43	111.27
18	2	610	CLA	O2D-CGD-CBD	4.02	118.42	111.27
18	A	843	CLA	O2D-CGD-CBD	4.02	118.40	111.27
18	4	602	CLA	O2D-CGD-CBD	4.01	118.39	111.27
18	A	802	CLA	O2D-CGD-CBD	4.01	118.39	111.27
18	A	832	CLA	O2D-CGD-CBD	4.00	118.38	111.27
18	2	608	CLA	O2D-CGD-CBD	3.99	118.36	111.27
18	G	203	CLA	O2D-CGD-CBD	3.99	118.36	111.27
18	A	842	CLA	O2D-CGD-CBD	3.99	118.35	111.27
18	B	802	CLA	O2D-CGD-CBD	3.98	118.35	111.27
19	1	615	LUT	C15-C35-C34	3.98	131.63	123.47
19	1	615	LUT	C19-C9-C10	-3.98	117.35	122.92
18	1	603	CLA	O2D-CGD-CBD	3.98	118.34	111.27
18	L	302	CLA	O2D-CGD-CBD	3.97	118.33	111.27
18	A	812	CLA	O2D-CGD-CBD	3.97	118.32	111.27
18	A	821	CLA	O2D-CGD-CBD	3.97	118.31	111.27
18	2	613	CLA	O2D-CGD-CBD	3.96	118.30	111.27
18	2	609	CLA	O2D-CGD-CBD	3.96	118.30	111.27
18	A	836	CLA	O2D-CGD-CBD	3.95	118.29	111.27
18	A	828	CLA	O2D-CGD-CBD	3.95	118.28	111.27
18	A	808	CLA	O2D-CGD-CBD	3.94	118.27	111.27
18	A	817	CLA	O2D-CGD-CBD	3.94	118.26	111.27
18	B	810	CLA	O2D-CGD-CBD	3.93	118.25	111.27
18	B	831	CLA	O2D-CGD-CBD	3.93	118.25	111.27
19	2	615	LUT	C19-C9-C10	-3.93	117.42	122.92
20	4	617	XAT	C7-C8-C9	3.93	131.62	125.53
18	B	802	CLA	C3B-C4B-NB	-3.92	106.87	110.52
18	B	838	CLA	O2D-CGD-CBD	3.92	118.23	111.27
18	A	834	CLA	O2D-CGD-CBD	3.92	118.23	111.27
19	3	614	LUT	C19-C9-C10	-3.91	117.45	122.92
18	3	604	CLA	O2D-CGD-CBD	3.90	118.19	111.27
18	3	610	CLA	O2D-CGD-CBD	3.89	118.18	111.27
18	A	811	CLA	O2D-CGD-CBD	3.89	118.17	111.27
18	L	304	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	K	202	CLA	O2D-CGD-CBD	3.88	118.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	613	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	B	829	CLA	O2D-CGD-CBD	3.88	118.17	111.27
18	B	836	CLA	O2D-CGD-CBD	3.88	118.16	111.27
18	B	832	CLA	C3B-C4B-NB	-3.88	106.92	110.52
18	A	810	CLA	O2D-CGD-CBD	3.87	118.15	111.27
18	B	820	CLA	O2D-CGD-CBD	3.87	118.15	111.27
18	1	614	CLA	O2D-CGD-CBD	3.87	118.14	111.27
18	1	610	CLA	O2D-CGD-CBD	3.86	118.13	111.27
18	A	807	CLA	O2D-CGD-CBD	3.86	118.13	111.27
18	B	818	CLA	O2D-CGD-CBD	3.86	118.12	111.27
19	3	614	LUT	C40-C33-C34	-3.86	117.52	122.92
19	3	614	LUT	C32-C33-C34	3.85	124.85	118.94
19	4	616	LUT	C19-C9-C10	-3.84	117.54	122.92
18	A	840	CLA	O2D-CGD-CBD	3.84	118.09	111.27
19	1	619	LUT	C39-C29-C30	-3.83	117.55	122.92
18	2	612	CLA	O2D-CGD-CBD	3.83	118.07	111.27
19	4	616	LUT	C39-C29-C30	-3.83	117.56	122.92
18	1	611	CLA	O2D-CGD-CBD	3.83	118.07	111.27
19	1	615	LUT	C39-C29-C30	-3.82	117.58	122.92
18	B	824	CLA	O2D-CGD-CBD	3.82	118.05	111.27
18	B	822	CLA	C3B-C4B-NB	-3.80	106.99	110.52
19	3	614	LUT	C28-C29-C30	3.79	124.76	118.94
18	2	602	CLA	O2D-CGD-CBD	3.79	118.00	111.27
18	B	820	CLA	C3B-C4B-NB	-3.78	107.00	110.52
18	1	602	CLA	O2D-CGD-CBD	3.78	117.98	111.27
18	B	834	CLA	O2D-CGD-CBD	3.77	117.97	111.27
18	B	805	CLA	O2D-CGD-CBD	3.77	117.97	111.27
18	A	826	CLA	C3B-C4B-NB	-3.77	107.02	110.52
18	4	609	CLA	C3B-C4B-NB	-3.77	107.02	110.52
18	3	609	CLA	O2D-CGD-CBD	3.77	117.96	111.27
18	1	612	CLA	O2D-CGD-CBD	3.76	117.96	111.27
18	A	801	CLA	O2D-CGD-CBD	3.76	117.96	111.27
18	A	835	CLA	O2D-CGD-CBD	3.76	117.96	111.27
18	2	604	CLA	O2D-CGD-CBD	3.76	117.94	111.27
18	B	817	CLA	O2D-CGD-CBD	3.75	117.94	111.27
18	4	614	CLA	O2D-CGD-CBD	3.75	117.93	111.27
18	3	603	CLA	O2D-CGD-CBD	3.74	117.91	111.27
17	2	607	CHL	CBC-CAC-C3C	-3.73	107.41	112.88
19	2	615	LUT	C39-C29-C30	-3.72	117.72	122.92
18	B	811	CLA	C3B-C4B-NB	-3.71	107.07	110.52
18	B	829	CLA	C3B-C4B-NB	-3.71	107.08	110.52
18	A	810	CLA	C3B-C4B-NB	-3.70	107.08	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	814	CLA	C3B-C4B-NB	-3.69	107.09	110.52
18	B	813	CLA	O2D-CGD-CBD	3.68	117.81	111.27
18	A	802	CLA	C3B-C4B-NB	-3.68	107.11	110.52
18	A	822	CLA	O2D-CGD-CBD	3.67	117.80	111.27
18	A	831	CLA	C3B-C4B-NB	-3.67	107.11	110.52
18	A	828	CLA	C3B-C4B-NB	-3.67	107.11	110.52
19	2	615	LUT	C15-C35-C34	3.66	130.98	123.47
18	B	825	CLA	C3B-C4B-NB	-3.66	107.12	110.52
18	1	602	CLA	C3B-C4B-NB	-3.65	107.13	110.52
18	F	303	CLA	O2D-CGD-CBD	3.64	117.73	111.27
18	2	611	CLA	O2D-CGD-CBD	3.63	117.72	111.27
18	B	806	CLA	C3B-C4B-NB	-3.63	107.15	110.52
18	3	607	CLA	O2D-CGD-CBD	3.63	117.71	111.27
18	K	203	CLA	O2D-CGD-CBD	3.63	117.71	111.27
18	A	815	CLA	C3B-C4B-NB	-3.62	107.16	110.52
18	4	602	CLA	C3B-C4B-NB	-3.62	107.16	110.52
18	3	617	CLA	C3B-C4B-NB	-3.62	107.16	110.52
18	4	603	CLA	O2D-CGD-CBD	3.62	117.69	111.27
18	A	840	CLA	C3B-C4B-NB	-3.61	107.16	110.52
18	A	834	CLA	C3B-C4B-NB	-3.61	107.16	110.52
18	1	614	CLA	C3B-C4B-NB	-3.61	107.17	110.52
17	4	615	CHL	CBC-CAC-C3C	-3.60	107.60	112.88
18	A	837	CLA	C4-C3-C5	-3.60	111.86	115.98
17	4	606	CHL	CAA-C2A-C3A	-3.60	102.91	112.78
18	A	806	CLA	C3B-C4B-NB	-3.60	107.18	110.52
18	B	821	CLA	C3B-C4B-NB	-3.60	107.18	110.52
18	A	819	CLA	C3B-C4B-NB	-3.59	107.19	110.52
18	A	803	CLA	C3B-C4B-NB	-3.58	107.19	110.52
18	B	836	CLA	C3B-C4B-NB	-3.58	107.20	110.52
18	A	822	CLA	C3B-C4B-NB	-3.57	107.20	110.52
18	A	814	CLA	O2D-CGD-CBD	3.56	117.59	111.27
18	A	808	CLA	C3B-C4B-NB	-3.56	107.21	110.52
17	2	601	CHL	CBC-CAC-C3C	-3.55	107.68	112.88
18	A	812	CLA	C3B-C4B-NB	-3.55	107.22	110.52
18	A	830	CLA	C3B-C4B-NB	-3.55	107.23	110.52
18	B	818	CLA	C3B-C4B-NB	-3.55	107.23	110.52
18	B	830	CLA	C3B-C4B-NB	-3.54	107.23	110.52
18	B	809	CLA	C3B-C4B-NB	-3.54	107.23	110.52
17	4	615	CHL	CAB-C3B-C2B	-3.54	117.75	124.69
18	A	832	CLA	C3B-C4B-NB	-3.54	107.23	110.52
18	L	303	CLA	C3B-C4B-NB	-3.53	107.24	110.52
18	2	608	CLA	C3B-C4B-NB	-3.52	107.25	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	304	CLA	O2D-CGD-CBD	3.52	117.53	111.27
17	1	606	CHL	OBD-CAD-CBD	-3.52	120.66	125.82
18	B	813	CLA	C3B-C4B-NB	-3.51	107.26	110.52
18	B	827	CLA	C3B-C4B-NB	-3.51	107.26	110.52
18	2	602	CLA	C3B-C4B-NB	-3.50	107.27	110.52
18	1	609	CLA	C3B-C4B-NB	-3.50	107.27	110.52
18	A	818	CLA	C3B-C4B-NB	-3.49	107.28	110.52
18	A	801	CLA	C3B-C4B-NB	-3.49	107.28	110.52
18	B	833	CLA	C3B-C4B-NB	-3.49	107.28	110.52
18	3	605	CLA	CHD-C1D-ND	-3.48	121.25	124.45
18	B	816	CLA	C3B-C4B-NB	-3.48	107.28	110.52
18	B	822	CLA	O2D-CGD-CBD	3.48	117.45	111.27
18	A	824	CLA	C3B-C4B-NB	-3.48	107.29	110.52
18	3	602	CLA	C3B-C4B-NB	-3.48	107.29	110.52
18	A	807	CLA	C3B-C4B-NB	-3.48	107.29	110.52
18	A	829	CLA	C3B-C4B-NB	-3.48	107.29	110.52
18	4	608	CLA	C3B-C4B-NB	-3.47	107.29	110.52
18	B	803	CLA	C3B-C4B-NB	-3.47	107.30	110.52
18	B	815	CLA	C3B-C4B-NB	-3.47	107.30	110.52
18	A	803	CLA	CHD-C1D-ND	-3.46	121.27	124.45
18	B	817	CLA	C3B-C4B-NB	-3.46	107.30	110.52
17	2	607	CHL	CMA-C3A-C4A	-3.46	106.80	114.38
17	4	605	CHL	CAA-C2A-C3A	-3.46	103.30	112.78
18	4	604	CLA	O2D-CGD-CBD	3.45	117.40	111.27
17	2	606	CHL	CMA-C3A-C4A	-3.45	106.82	114.38
18	2	609	CLA	C3B-C4B-NB	-3.45	107.32	110.52
18	B	835	CLA	C3B-C4B-NB	-3.45	107.32	110.52
17	2	614	CHL	CBC-CAC-C3C	-3.43	107.85	112.88
18	2	604	CLA	C3B-C4B-NB	-3.43	107.33	110.52
18	B	828	CLA	C3B-C4B-NB	-3.43	107.33	110.52
17	1	601	CHL	OBD-CAD-CBD	-3.42	120.80	125.82
18	A	821	CLA	C3B-C4B-NB	-3.42	107.34	110.52
18	F	301	CLA	C3B-C4B-NB	-3.42	107.34	110.52
18	A	843	CLA	O2A-CGA-CBA	3.42	122.64	111.91
20	4	617	XAT	O24-C25-C24	-3.42	110.82	113.38
17	1	601	CHL	C1-C2-C3	3.41	131.95	126.04
19	1	619	LUT	C20-C13-C14	-3.41	118.15	122.92
18	A	838	CLA	C3B-C4B-NB	-3.41	107.35	110.52
18	3	613	CLA	C3B-C4B-NB	-3.41	107.36	110.52
18	B	804	CLA	C3B-C4B-NB	-3.40	107.36	110.52
18	A	809	CLA	C3B-C4B-NB	-3.39	107.37	110.52
18	A	831	CLA	O2A-CGA-CBA	3.39	122.56	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	605	CHL	CBC-CAC-C3C	-3.39	107.92	112.88
18	B	840	CLA	C3B-C4B-NB	-3.38	107.38	110.52
20	3	615	XAT	O24-C25-C24	-3.38	110.84	113.38
18	G	203	CLA	C3B-C4B-NB	-3.37	107.39	110.52
18	3	606	CLA	C3B-C4B-NB	-3.37	107.39	110.52
18	B	814	CLA	C3B-C4B-NB	-3.36	107.39	110.52
18	B	807	CLA	O2A-CGA-CBA	3.36	122.46	111.91
18	1	610	CLA	C3B-C4B-NB	-3.36	107.40	110.52
18	A	835	CLA	C3B-C4B-NB	-3.36	107.40	110.52
18	A	827	CLA	C3B-C4B-NB	-3.36	107.40	110.52
17	2	605	CHL	CMA-C3A-C4A	-3.36	107.02	114.38
18	H	201	CLA	C3B-C4B-NB	-3.36	107.40	110.52
18	B	801	CLA	C3B-C4B-NB	-3.36	107.40	110.52
18	4	614	CLA	O2A-CGA-CBA	3.35	122.44	111.91
18	2	603	CLA	C3B-C4B-NB	-3.35	107.40	110.52
18	H	201	CLA	O2D-CGD-CBD	3.35	117.23	111.27
17	2	605	CHL	OBD-CAD-CBD	-3.35	120.90	125.82
18	4	601	CLA	C3B-C4B-NB	-3.35	107.40	110.52
18	3	609	CLA	C3B-C4B-NB	-3.35	107.41	110.52
18	A	824	CLA	O2D-CGD-CBD	3.35	117.22	111.27
18	A	805	CLA	C3B-C4B-NB	-3.35	107.41	110.52
18	B	812	CLA	C3B-C4B-NB	-3.34	107.42	110.52
17	4	606	CHL	CMA-C3A-C4A	-3.34	107.06	114.38
18	2	612	CLA	C3B-C4B-NB	-3.34	107.42	110.52
18	B	808	CLA	C3B-C4B-NB	-3.34	107.42	110.52
17	4	605	CHL	CMA-C3A-C4A	-3.34	107.07	114.38
17	3	616	CHL	CMA-C3A-C4A	-3.33	107.09	114.38
18	1	611	CLA	C3B-C4B-NB	-3.33	107.43	110.52
18	F	304	CLA	C3B-C4B-NB	-3.32	107.43	110.52
17	4	607	CHL	CMA-C3A-C4A	-3.32	107.10	114.38
18	A	813	CLA	C3B-C4B-NB	-3.32	107.43	110.52
18	F	303	CLA	C3B-C4B-NB	-3.32	107.44	110.52
17	2	606	CHL	OBD-CAD-CBD	-3.32	120.95	125.82
21	J	101	BCR	C23-C24-C25	3.31	136.51	127.20
18	B	831	CLA	C3B-C4B-NB	-3.31	107.44	110.52
18	4	604	CLA	C3B-C4B-NB	-3.31	107.44	110.52
18	1	613	CLA	C3B-C4B-NB	-3.31	107.44	110.52
18	2	613	CLA	C3B-C4B-NB	-3.31	107.45	110.52
18	4	614	CLA	C3B-C4B-NB	-3.31	107.45	110.52
17	2	614	CHL	CMA-C3A-C4A	-3.30	107.14	114.38
18	A	841	CLA	C3B-C4B-NB	-3.30	107.45	110.52
18	B	802	CLA	C1-C2-C3	3.30	131.75	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	3	608	CLA	C3B-C4B-NB	-3.30	107.45	110.52
18	1	605	CLA	C3B-C4B-NB	-3.30	107.45	110.52
17	4	607	CHL	OBD-CAD-CBD	-3.30	120.99	125.82
18	B	819	CLA	C3B-C4B-NB	-3.30	107.46	110.52
18	B	838	CLA	C3B-C4B-NB	-3.29	107.46	110.52
18	B	834	CLA	C3B-C4B-NB	-3.29	107.46	110.52
20	2	616	XAT	O4-C5-C4	-3.29	110.91	113.38
18	A	823	CLA	C3B-C4B-NB	-3.29	107.47	110.52
18	1	604	CLA	C3B-C4B-NB	-3.28	107.47	110.52
20	1	616	XAT	C7-C8-C9	3.28	130.62	125.53
18	B	832	CLA	CHD-C1D-ND	-3.28	121.44	124.45
18	B	816	CLA	C12-C11-C10	-3.27	102.05	113.62
18	B	824	CLA	C3B-C4B-NB	-3.27	107.48	110.52
18	L	304	CLA	C3B-C4B-NB	-3.27	107.48	110.52
18	B	805	CLA	C3B-C4B-NB	-3.27	107.49	110.52
18	B	839	CLA	C3B-C4B-NB	-3.26	107.49	110.52
18	A	820	CLA	C3B-C4B-NB	-3.25	107.50	110.52
17	2	606	CHL	CBC-CAC-C3C	-3.25	108.12	112.88
17	4	615	CHL	CMA-C3A-C4A	-3.25	107.27	114.38
18	2	610	CLA	C3B-C4B-NB	-3.24	107.51	110.52
18	A	839	CLA	C3B-C4B-NB	-3.24	107.51	110.52
18	B	826	CLA	C3B-C4B-NB	-3.24	107.51	110.52
18	1	612	CLA	C3B-C4B-NB	-3.23	107.51	110.52
17	1	606	CHL	CMA-C3A-C4A	-3.23	107.29	114.38
18	1	607	CLA	C3B-C4B-NB	-3.23	107.52	110.52
18	4	611	CLA	C3B-C4B-NB	-3.23	107.52	110.52
17	4	605	CHL	C1-C2-C3	3.23	131.63	126.04
17	2	601	CHL	CMA-C3A-C4A	-3.22	107.32	114.38
18	3	603	CLA	O2A-CGA-CBA	3.22	122.02	111.91
18	A	817	CLA	C3B-C4B-NB	-3.22	107.53	110.52
18	1	608	CLA	C3B-C4B-NB	-3.22	107.53	110.52
19	4	616	LUT	C40-C33-C34	-3.21	118.42	122.92
18	A	821	CLA	CHD-C1D-ND	-3.21	121.50	124.45
18	A	811	CLA	C3B-C4B-NB	-3.21	107.54	110.52
18	A	816	CLA	C3B-C4B-NB	-3.21	107.54	110.52
18	4	609	CLA	O2A-CGA-CBA	3.21	121.97	111.91
17	3	616	CHL	OBD-CAD-CBD	-3.21	121.12	125.82
17	2	601	CHL	C1C-CHC-C4B	3.20	126.34	115.73
18	B	802	CLA	CHD-C1D-ND	-3.20	121.51	124.45
18	G	202	CLA	C3B-C4B-NB	-3.20	107.55	110.52
18	K	201	CLA	C3B-C4B-NB	-3.20	107.55	110.52
17	2	607	CHL	OBD-CAD-CBD	-3.20	121.13	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	1	606	CHL	C1C-CHC-C4B	3.20	126.33	115.73
17	2	607	CHL	CAA-C2A-C3A	-3.19	104.03	112.78
18	A	804	CLA	C3B-C4B-NB	-3.19	107.55	110.52
17	4	606	CHL	OBD-CAD-CBD	-3.19	121.14	125.82
17	1	601	CHL	CMA-C3A-C4A	-3.19	107.39	114.38
18	1	610	CLA	O2A-CGA-CBA	3.19	121.92	111.91
18	A	834	CLA	O2A-CGA-CBA	3.19	121.92	111.91
18	A	833	CLA	O2A-CGA-CBA	3.19	121.91	111.91
18	1	603	CLA	C3B-C4B-NB	-3.19	107.56	110.52
18	3	605	CLA	C3B-C4B-NB	-3.19	107.56	110.52
18	A	833	CLA	C3B-C4B-NB	-3.19	107.56	110.52
17	2	601	CHL	CAA-C2A-C3A	-3.18	104.06	112.78
18	A	811	CLA	O2A-CGA-CBA	3.18	121.89	111.91
18	A	801	CLA	O2A-CGA-CBA	3.18	121.88	111.91
18	4	613	CLA	C3B-C4B-NB	-3.18	107.57	110.52
17	4	607	CHL	C1-C2-C3	3.17	131.88	126.75
18	4	610	CLA	C3B-C4B-NB	-3.17	107.58	110.52
18	A	821	CLA	O2A-CGA-CBA	3.17	121.85	111.91
18	A	825	CLA	O2A-CGA-CBA	3.17	121.85	111.91
18	1	609	CLA	O2A-CGA-CBA	3.17	121.85	111.91
18	4	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	B	838	CLA	O2A-CGA-CBA	3.16	121.83	111.91
18	B	837	CLA	C3B-C4B-NB	-3.16	107.58	110.52
18	2	609	CLA	CHD-C1D-ND	-3.16	121.55	124.45
18	B	821	CLA	O2A-CGA-CBA	3.16	121.81	111.91
18	B	807	CLA	C3B-C4B-NB	-3.16	107.59	110.52
18	B	827	CLA	O2A-CGA-CBA	3.15	121.80	111.91
18	A	813	CLA	O2A-CGA-CBA	3.15	121.79	111.91
17	1	601	CHL	O2A-CGA-CBA	3.15	121.79	111.91
18	A	842	CLA	C3B-C4B-NB	-3.15	107.59	110.52
18	A	830	CLA	O2A-CGA-CBA	3.14	121.77	111.91
18	B	836	CLA	O2A-CGA-CBA	3.14	121.77	111.91
18	A	854	CLA	O2A-CGA-CBA	3.14	121.77	111.91
18	A	817	CLA	O2A-CGA-CBA	3.14	121.76	111.91
18	A	836	CLA	C3B-C4B-NB	-3.14	107.60	110.52
18	J	102	CLA	C3B-C4B-NB	-3.14	107.60	110.52
19	1	615	LUT	C40-C33-C34	-3.14	118.53	122.92
18	1	604	CLA	O2A-CGA-CBA	3.13	121.74	111.91
18	A	803	CLA	O2A-CGA-CBA	3.13	121.74	111.91
18	A	854	CLA	C3B-C4B-NB	-3.13	107.61	110.52
18	2	602	CLA	O2A-CGA-CBA	3.13	121.74	111.91
17	1	601	CHL	CBC-CAC-C3C	-3.13	108.30	112.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
18	A	838	CLA	O2A-CGA-CBA	3.13	121.73	111.91
18	B	825	CLA	O2A-CGA-CBA	3.13	121.72	111.91
18	3	607	CLA	C3B-C4B-NB	-3.13	107.61	110.52
18	K	202	CLA	C3B-C4B-NB	-3.12	107.62	110.52
18	B	814	CLA	O2A-CGA-CBA	3.12	121.70	111.91
18	A	831	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	B	831	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	A	826	CLA	CHD-C1D-ND	-3.12	121.59	124.45
18	2	612	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	A	837	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	B	840	CLA	O2A-CGA-CBA	3.11	121.67	111.91
18	A	811	CLA	CHD-C1D-ND	-3.11	121.59	124.45
17	1	601	CHL	C1C-CHC-C4B	3.11	126.03	115.73
18	4	608	CLA	CHD-C1D-ND	-3.11	121.60	124.45
18	L	302	CLA	C3B-C4B-NB	-3.10	107.64	110.52
18	B	836	CLA	C1-C2-C3	3.10	131.41	126.04
18	A	843	CLA	CHD-C1D-ND	-3.10	121.60	124.45
18	4	612	CLA	C3B-C4B-NB	-3.10	107.64	110.52
17	4	615	CHL	C1C-CHC-C4B	3.10	126.01	115.73
18	A	826	CLA	O2A-CGA-CBA	3.10	121.63	111.91
18	3	604	CLA	C3B-C4B-NB	-3.10	107.64	110.52
18	2	609	CLA	O2A-CGA-CBA	3.10	121.62	111.91
18	A	824	CLA	O2A-CGA-CBA	3.09	121.61	111.91
18	A	825	CLA	C3B-C4B-NB	-3.09	107.65	110.52
18	K	203	CLA	C3B-C4B-NB	-3.09	107.65	110.52
17	4	605	CHL	C1C-CHC-C4B	3.09	125.95	115.73
18	B	810	CLA	CHD-C1D-ND	-3.08	121.62	124.45
18	3	611	CLA	C3B-C4B-NB	-3.08	107.66	110.52
18	3	612	CLA	C3B-C4B-NB	-3.08	107.66	110.52
19	2	615	LUT	C40-C33-C34	-3.08	118.61	122.92
17	2	614	CHL	C1C-CHC-C4B	3.07	125.92	115.73
17	2	601	CHL	C1A-CHA-C4D	3.07	124.11	118.98
18	B	805	CLA	O2A-CGA-CBA	3.07	121.55	111.91
18	A	806	CLA	O2A-CGA-CBA	3.07	121.55	111.91
18	3	610	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	B	829	CLA	CHD-C1D-ND	-3.07	121.63	124.45
18	B	828	CLA	O2A-CGA-CBA	3.07	121.54	111.91
18	B	821	CLA	CHD-C1D-ND	-3.07	121.64	124.45
18	A	808	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	A	843	CLA	C3B-C4B-NB	-3.07	107.67	110.52
18	B	817	CLA	O2A-CGA-CBA	3.07	121.53	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	815	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	808	CLA	O2A-CGA-CBA	3.07	121.53	111.91
18	B	812	CLA	O2A-CGA-CBA	3.06	121.52	111.91
18	A	818	CLA	O2A-CGA-CBA	3.06	121.52	111.91
18	A	810	CLA	O2A-CGA-CBA	3.06	121.51	111.91
17	2	606	CHL	C1C-CHC-C4B	3.06	125.86	115.73
18	H	201	CLA	C4-C3-C5	-3.06	112.49	115.98
18	B	819	CLA	O2A-CGA-CBA	3.05	121.49	111.91
18	G	204	CLA	C3B-C4B-NB	-3.05	107.68	110.52
18	B	822	CLA	CHD-C1D-ND	-3.05	121.65	124.45
18	3	608	CLA	CHD-C1D-ND	-3.05	121.65	124.45
19	1	619	LUT	C12-C13-C14	3.05	123.62	118.94
18	4	612	CLA	O2A-CGA-CBA	3.05	121.47	111.91
18	1	611	CLA	CHD-C1D-ND	-3.04	121.66	124.45
17	4	606	CHL	C1C-CHC-C4B	3.04	125.80	115.73
19	2	615	LUT	C35-C15-C14	3.03	129.69	123.47
18	B	806	CLA	O2A-CGA-CBA	3.03	121.41	111.91
17	2	614	CHL	C4C-CHD-C1D	3.03	125.76	115.73
18	A	802	CLA	CHD-C1D-ND	-3.03	121.67	124.45
17	1	601	CHL	C4C-CHD-C1D	3.02	125.75	115.73
17	1	601	CHL	CAA-C2A-C3A	-3.02	104.50	112.78
18	B	839	CLA	O2A-CGA-CBA	3.02	121.38	111.91
18	A	837	CLA	C3B-C4B-NB	-3.02	107.72	110.52
17	4	607	CHL	C1C-CHC-C4B	3.02	125.72	115.73
18	B	815	CLA	CHD-C1D-ND	-3.02	121.68	124.45
18	A	812	CLA	O2A-CGA-CBA	3.02	121.37	111.91
19	3	614	LUT	C20-C13-C14	-3.01	118.70	122.92
18	F	303	CLA	CHD-C1D-ND	-3.01	121.69	124.45
18	B	835	CLA	O2A-CGA-CBA	3.01	121.35	111.91
19	1	619	LUT	C40-C33-C34	-3.01	118.71	122.92
18	A	842	CLA	O2A-CGA-CBA	3.01	121.35	111.91
17	4	615	CHL	C4C-CHD-C1D	3.01	125.69	115.73
17	2	606	CHL	C4C-CHD-C1D	3.00	125.69	115.73
18	1	612	CLA	O2A-CGA-CBA	3.00	121.34	111.91
18	A	808	CLA	CHD-C1D-ND	-3.00	121.69	124.45
17	4	615	CHL	OBD-CAD-CBD	-3.00	121.42	125.82
17	3	616	CHL	C4C-CHD-C1D	3.00	125.68	115.73
19	2	615	LUT	C20-C13-C14	-3.00	118.72	122.92
18	B	810	CLA	O2A-CGA-CBA	3.00	121.31	111.91
18	A	824	CLA	CHD-C1D-ND	-2.99	121.70	124.45
17	2	605	CHL	C1C-CHC-C4B	2.99	125.65	115.73
18	2	604	CLA	CHD-C1D-ND	-2.99	121.70	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	823	CLA	CHD-C1D-ND	-2.99	121.70	124.45
18	A	839	CLA	O2A-CGA-CBA	2.99	121.30	111.91
18	B	836	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	F	301	CLA	O2A-CGA-CBA	2.99	121.28	111.91
18	4	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
18	A	841	CLA	O2A-CGA-CBA	2.98	121.28	111.91
17	4	605	CHL	C1A-CHA-C4D	2.98	123.96	118.98
18	A	833	CLA	CHD-C1D-ND	-2.98	121.72	124.45
17	2	601	CHL	CHA-C1A-C2A	-2.98	126.31	133.31
18	B	824	CLA	O2A-CGA-CBA	2.98	121.25	111.91
17	3	616	CHL	CAA-C2A-C3A	-2.97	104.63	112.78
18	A	834	CLA	CHD-C1D-ND	-2.97	121.72	124.45
18	3	603	CLA	C3B-C4B-NB	-2.97	107.76	110.52
18	A	818	CLA	C12-C11-C10	-2.97	103.12	113.62
17	4	607	CHL	C4C-CHD-C1D	2.97	125.56	115.73
18	B	814	CLA	CHD-C1D-ND	-2.97	121.73	124.45
17	2	607	CHL	C4C-CHD-C1D	2.97	125.56	115.73
18	B	833	CLA	O2A-CGA-CBA	2.97	121.22	111.91
18	2	604	CLA	O2A-CGA-CBA	2.96	121.21	111.91
18	A	827	CLA	O2A-CGA-CBA	2.96	121.21	111.91
18	B	823	CLA	C3B-C4B-NB	-2.96	107.77	110.52
18	1	608	CLA	CHD-C1D-ND	-2.96	121.73	124.45
18	B	801	CLA	CHD-C1D-ND	-2.96	121.73	124.45
18	2	602	CLA	CHD-C1D-ND	-2.96	121.74	124.45
18	B	816	CLA	O2A-CGA-CBA	2.96	121.19	111.91
18	3	613	CLA	CHD-C1D-ND	-2.96	121.74	124.45
17	3	616	CHL	C3C-C4C-NC	-2.95	108.49	115.01
18	2	611	CLA	C3B-C4B-NB	-2.95	107.78	110.52
18	B	823	CLA	O2A-CGA-CBA	2.95	121.17	111.91
18	1	602	CLA	C1-C2-C3	2.95	131.15	126.04
19	1	615	LUT	C20-C13-C14	-2.95	118.79	122.92
17	1	606	CHL	C4C-CHD-C1D	2.95	125.50	115.73
18	A	840	CLA	CHD-C1D-ND	-2.95	121.74	124.45
25	B	841	PQN	C11-C3-C4	-2.95	115.35	118.50
17	4	606	CHL	C4C-CHD-C1D	2.94	125.48	115.73
18	B	822	CLA	O2A-CGA-CBA	2.94	121.13	111.91
17	4	606	CHL	C1A-CHA-C4D	2.94	123.89	118.98
17	4	615	CHL	C1A-CHA-C4D	2.94	123.89	118.98
18	1	602	CLA	O2A-CGA-CBA	2.94	121.13	111.91
17	2	607	CHL	C1C-CHC-C4B	2.94	125.47	115.73
18	B	813	CLA	CHD-C1D-ND	-2.94	121.75	124.45
18	B	809	CLA	O2A-CGA-CBA	2.94	121.13	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	607	CHL	O2A-CGA-CBA	2.94	121.13	111.91
18	4	610	CLA	O2A-CGA-CBA	2.94	121.12	111.91
17	1	606	CHL	CMA-C3A-C2A	-2.93	109.25	116.10
18	A	807	CLA	O2A-CGA-CBA	2.93	121.11	111.91
17	3	616	CHL	C1C-CHC-C4B	2.93	125.45	115.73
18	A	827	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	L	303	CLA	O2A-CGA-CBA	2.93	121.10	111.91
18	1	608	CLA	O2A-CGA-CBA	2.93	121.10	111.91
18	B	825	CLA	CHD-C1D-ND	-2.93	121.76	124.45
18	3	605	CLA	O2A-CGA-CBA	2.92	121.08	111.91
18	A	806	CLA	CHD-C1D-ND	-2.92	121.77	124.45
18	A	828	CLA	O2A-CGA-CBA	2.92	121.07	111.91
18	A	801	CLA	CHD-C1D-ND	-2.92	121.77	124.45
17	2	605	CHL	C4C-CHD-C1D	2.92	125.39	115.73
18	A	819	CLA	CHD-C1D-ND	-2.92	121.78	124.45
18	3	602	CLA	O2A-CGA-CBA	2.91	121.05	111.91
17	2	601	CHL	C3C-C4C-NC	-2.91	108.58	115.01
18	1	602	CLA	CHD-C1D-ND	-2.91	121.78	124.45
18	A	836	CLA	CHD-C1D-ND	-2.91	121.78	124.45
17	2	605	CHL	C1A-CHA-C4D	2.91	123.84	118.98
18	B	817	CLA	CHD-C1D-ND	-2.91	121.78	124.45
17	2	614	CHL	C3C-C4C-NC	-2.90	108.60	115.01
18	2	611	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	A	837	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	2	603	CLA	CHD-C1D-ND	-2.90	121.79	124.45
18	B	820	CLA	O2A-CGA-CBA	2.90	121.00	111.91
17	4	607	CHL	C3C-C4C-NC	-2.89	108.63	115.01
18	3	617	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	4	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	F	301	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	B	804	CLA	CHD-C1D-ND	-2.89	121.80	124.45
18	B	838	CLA	C1-C2-C3	2.89	131.03	126.04
18	B	810	CLA	CAB-C3B-C2B	-2.88	116.12	123.59
17	2	607	CHL	C3C-C4C-NC	-2.88	108.66	115.01
18	B	801	CLA	O2A-CGA-CBA	2.88	120.94	111.91
18	1	603	CLA	O2A-CGA-CBA	2.88	120.93	111.91
18	A	838	CLA	CHD-C1D-ND	-2.87	121.81	124.45
18	A	819	CLA	O2A-CGA-CBA	2.87	120.92	111.91
17	2	606	CHL	C3C-C4C-NC	-2.87	108.67	115.01
18	J	102	CLA	CHD-C1D-ND	-2.87	121.81	124.45
17	4	615	CHL	C3C-C4C-NC	-2.87	108.67	115.01
17	2	607	CHL	C1-C2-C3	2.87	131.40	126.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	842	CLA	CHD-C1D-ND	-2.87	121.82	124.45
18	B	824	CLA	CHD-C1D-ND	-2.87	121.82	124.45
25	A	844	PQN	C11-C3-C4	-2.87	115.43	118.50
18	H	201	CLA	O2A-CGA-CBA	2.87	120.90	111.91
18	A	829	CLA	O2A-CGA-CBA	2.86	120.89	111.91
17	1	601	CHL	C3C-C4C-NC	-2.86	108.69	115.01
18	B	803	CLA	CHD-C1D-ND	-2.86	121.82	124.45
18	A	817	CLA	C1-C2-C3	2.86	130.99	126.04
17	1	606	CHL	C3C-C4C-NC	-2.86	108.70	115.01
18	A	830	CLA	C1-C2-C3	2.86	130.99	126.04
18	A	802	CLA	O2A-CGA-CBA	2.86	120.88	111.91
18	A	804	CLA	O2A-CGA-CBA	2.86	120.87	111.91
18	4	603	CLA	C3B-C4B-NB	-2.86	107.86	110.52
18	A	825	CLA	CHD-C1D-ND	-2.86	121.83	124.45
18	B	809	CLA	CHD-C1D-ND	-2.86	121.83	124.45
18	A	810	CLA	CHD-C1D-ND	-2.86	121.83	124.45
18	A	841	CLA	CHD-C1D-ND	-2.86	121.83	124.45
20	2	616	XAT	C7-C8-C9	2.86	129.96	125.53
18	B	840	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	B	806	CLA	CHD-C1D-ND	-2.85	121.83	124.45
17	1	606	CHL	C1A-CHA-C4D	2.85	123.74	118.98
18	A	840	CLA	O2A-CGA-CBA	2.85	120.85	111.91
18	B	820	CLA	CHD-C1D-ND	-2.85	121.83	124.45
18	L	303	CLA	C1-C2-C3	2.85	130.97	126.04
18	A	828	CLA	C1-C2-C3	2.85	130.97	126.04
17	2	601	CHL	C4C-CHD-C1D	2.85	125.16	115.73
18	4	601	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	B	833	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	G	203	CLA	CHD-C1D-ND	-2.85	121.84	124.45
18	A	805	CLA	CHD-C1D-ND	-2.84	121.84	124.45
18	B	835	CLA	CHD-C1D-ND	-2.84	121.84	124.45
19	1	619	LUT	C15-C35-C34	2.84	129.29	123.47
18	A	809	CLA	O2A-CGA-CBA	2.84	120.82	111.91
17	4	607	CHL	CAA-C2A-C3A	-2.84	105.01	112.78
18	B	818	CLA	C1-C2-C3	2.84	130.95	126.04
19	3	614	LUT	C30-C31-C32	2.84	132.07	123.22
18	A	813	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	829	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	3	612	CLA	CHD-C1D-ND	-2.83	121.85	124.45
18	A	823	CLA	CHD-C1D-ND	-2.83	121.85	124.45
17	2	606	CHL	C1A-CHA-C4D	2.83	123.70	118.98
18	B	827	CLA	CHD-C1D-ND	-2.82	121.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	616	LUT	C20-C13-C14	-2.82	118.97	122.92
18	B	834	CLA	CHD-C1D-ND	-2.82	121.86	124.45
18	A	830	CLA	CHD-C1D-ND	-2.82	121.87	124.45
18	4	611	CLA	CHD-C1D-ND	-2.82	121.87	124.45
18	A	828	CLA	CHD-C1D-ND	-2.82	121.87	124.45
17	4	605	CHL	C3C-C4C-NC	-2.81	108.81	115.01
18	B	823	CLA	C1-C2-C3	2.81	130.90	126.04
17	2	614	CHL	C1A-CHA-C4D	2.81	123.67	118.98
18	3	609	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	A	818	CLA	CHD-C1D-ND	-2.81	121.88	124.45
18	B	828	CLA	CHD-C1D-ND	-2.81	121.88	124.45
17	4	605	CHL	C4C-CHD-C1D	2.80	125.02	115.73
18	L	304	CLA	CHD-C1D-ND	-2.80	121.88	124.45
18	2	608	CLA	CHD-C1D-ND	-2.80	121.88	124.45
18	A	811	CLA	C1-C2-C3	2.80	130.88	126.04
17	1	601	CHL	C1A-CHA-C4D	2.79	123.64	118.98
18	B	839	CLA	CHD-C1D-ND	-2.79	121.89	124.45
19	1	615	LUT	C35-C15-C14	2.79	129.19	123.47
18	B	837	CLA	O2A-CGA-CBA	2.79	120.66	111.91
18	1	612	CLA	CHD-C1D-ND	-2.79	121.89	124.45
18	B	826	CLA	O2A-CGA-CBA	2.79	120.65	111.91
18	3	602	CLA	CHD-C1D-ND	-2.78	121.89	124.45
18	B	831	CLA	O2A-CGA-CBA	2.78	120.63	111.91
18	L	303	CLA	CHD-C1D-ND	-2.78	121.90	124.45
17	2	607	CHL	O2A-CGA-CBA	2.78	120.63	111.91
18	1	610	CLA	CHD-C1D-ND	-2.77	121.90	124.45
18	B	825	CLA	C4-C3-C5	-2.77	110.60	115.27
18	4	602	CLA	O2A-CGA-CBA	2.77	120.61	111.91
18	2	610	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	A	814	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	A	812	CLA	C1-C2-C3	2.77	130.84	126.04
17	2	601	CHL	OBD-CAD-CBD	-2.77	121.76	125.82
18	K	203	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	H	201	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	F	304	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	1	613	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	B	818	CLA	CHD-C1D-ND	-2.77	121.91	124.45
18	2	602	CLA	C1-C2-C3	2.76	130.82	126.04
18	2	613	CLA	CHD-C1D-ND	-2.76	121.91	124.45
17	4	606	CHL	C3C-C4C-NC	-2.76	108.91	115.01
18	A	832	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	813	CLA	C1-C2-C3	2.76	130.82	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	812	CLA	CHD-C1D-ND	-2.76	121.92	124.45
18	B	813	CLA	O2A-CGA-CBA	2.76	120.57	111.91
17	4	605	CHL	OBD-CAD-CBD	-2.76	121.78	125.82
18	B	804	CLA	O2A-CGA-CBA	2.76	120.56	111.91
18	A	839	CLA	CHD-C1D-ND	-2.76	121.92	124.45
19	4	616	LUT	C32-C33-C34	2.76	123.17	118.94
18	A	854	CLA	CHD-C1D-ND	-2.75	121.92	124.45
18	B	801	CLA	C1-C2-C3	2.75	130.81	126.04
18	A	822	CLA	CHD-C1D-ND	-2.75	121.92	124.45
18	4	602	CLA	CHD-C1D-ND	-2.75	121.93	124.45
18	B	808	CLA	CHD-C1D-ND	-2.75	121.93	124.45
17	3	616	CHL	O1D-CGD-CBD	-2.75	120.17	124.74
18	3	603	CLA	CHD-C1D-ND	-2.75	121.93	124.45
18	1	607	CLA	CHD-C1D-ND	-2.74	121.93	124.45
18	A	809	CLA	CHD-C1D-ND	-2.74	121.93	124.45
18	3	607	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	1	604	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	A	804	CLA	C1-C2-C3	2.73	130.76	126.04
18	B	816	CLA	CHD-C1D-ND	-2.73	121.94	124.45
18	K	202	CLA	CHD-C1D-ND	-2.73	121.95	124.45
18	3	617	CLA	O2A-CGA-CBA	2.73	120.47	111.91
18	A	823	CLA	CMA-C3A-C2A	-2.73	109.73	116.10
18	B	830	CLA	CHD-C1D-ND	-2.73	121.95	124.45
18	A	817	CLA	CHD-C1D-ND	-2.73	121.95	124.45
17	4	607	CHL	CHA-C1A-C2A	-2.72	126.91	133.31
18	A	815	CLA	CHD-C1D-ND	-2.72	121.95	124.45
18	3	610	CLA	CHD-C1D-ND	-2.72	121.95	124.45
18	B	802	CLA	O2A-CGA-CBA	2.72	120.44	111.91
17	3	616	CHL	CHA-C1A-C2A	-2.72	126.93	133.31
18	3	606	CLA	CHD-C1D-ND	-2.71	121.96	124.45
18	1	605	CLA	CHD-C1D-ND	-2.71	121.96	124.45
18	1	610	CLA	C1-C2-C3	2.71	130.73	126.04
18	A	812	CLA	CHD-C1D-ND	-2.71	121.97	124.45
18	A	832	CLA	O2A-CGA-CBA	2.71	120.40	111.91
18	G	204	CLA	CHD-C1D-ND	-2.70	121.97	124.45
18	G	202	CLA	CHD-C1D-ND	-2.70	121.97	124.45
19	1	619	LUT	C39-C29-C28	2.69	122.32	118.08
18	A	804	CLA	CHD-C1D-ND	-2.69	121.98	124.45
18	B	804	CLA	C1-C2-C3	2.69	130.70	126.04
18	F	304	CLA	CMA-C3A-C2A	-2.69	109.82	116.10
18	4	604	CLA	CHD-C1D-ND	-2.69	121.99	124.45
20	1	616	XAT	O4-C5-C4	-2.68	111.37	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	4	606	CHL	CHA-C1A-C2A	-2.68	127.01	133.31
17	2	614	CHL	OBD-CAD-CBD	-2.68	121.89	125.82
18	2	612	CLA	CHD-C1D-ND	-2.68	121.99	124.45
18	3	613	CLA	CMA-C3A-C2A	-2.68	109.85	116.10
18	B	820	CLA	C1-C2-C3	2.68	130.67	126.04
18	B	805	CLA	CHD-C1D-ND	-2.67	122.00	124.45
18	B	837	CLA	CHD-C1D-ND	-2.67	122.00	124.45
19	1	615	LUT	C32-C33-C34	2.67	123.04	118.94
18	A	854	CLA	C1-C2-C3	2.67	131.07	126.75
17	4	605	CHL	O2A-CGA-CBA	2.66	120.27	111.91
18	A	819	CLA	CHB-C1B-NB	2.65	127.07	124.26
18	1	609	CLA	CHD-C1D-ND	-2.65	122.02	124.45
18	3	609	CLA	CMA-C3A-C2A	-2.65	109.91	116.10
18	B	821	CLA	C1-C2-C3	2.65	130.63	126.04
17	2	614	CHL	O1D-CGD-CBD	-2.65	120.33	124.74
18	K	201	CLA	CHD-C1D-ND	-2.65	122.02	124.45
18	3	612	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
18	4	602	CLA	C1-C2-C3	2.65	130.62	126.04
18	B	803	CLA	CMA-C3A-C2A	-2.65	109.92	116.10
18	A	820	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	B	811	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	3	611	CLA	CHD-C1D-ND	-2.64	122.03	124.45
18	4	614	CLA	CHD-C1D-ND	-2.63	122.04	124.45
21	A	847	BCR	C7-C8-C9	2.63	130.21	126.23
17	4	607	CHL	OMC-CMC-C2C	-2.62	120.83	125.03
17	1	601	CHL	CHA-C1A-C2A	-2.62	127.15	133.31
18	B	808	CLA	CHB-C1B-NB	2.62	127.03	124.26
18	A	835	CLA	CHD-C1D-ND	-2.62	122.05	124.45
18	4	613	CLA	CHD-C1D-ND	-2.61	122.05	124.45
18	4	612	CLA	CHD-C1D-ND	-2.61	122.06	124.45
18	L	302	CLA	CHD-C1D-ND	-2.60	122.06	124.45
18	B	827	CLA	C1-C2-C3	2.60	130.54	126.04
18	B	838	CLA	CHD-C1D-ND	-2.60	122.06	124.45
17	2	601	CHL	O1D-CGD-CBD	-2.60	120.41	124.74
18	B	833	CLA	C1-C2-C3	2.60	130.53	126.04
18	A	807	CLA	CHD-C1D-ND	-2.60	122.07	124.45
18	A	801	CLA	C1-C2-C3	2.59	130.53	126.04
17	2	601	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
18	4	603	CLA	O2A-CGA-CBA	2.58	122.33	114.03
18	B	817	CLA	CHB-C1B-NB	2.58	126.99	124.26
17	4	605	CHL	CHA-C1A-C2A	-2.58	127.25	133.31
18	F	301	CLA	C1-C2-C3	2.58	130.50	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	1	609	CLA	C1-C2-C3	2.58	130.50	126.04
18	B	818	CLA	O2A-CGA-CBA	2.57	119.99	111.91
18	2	604	CLA	C1-C2-C3	2.57	130.49	126.04
18	2	609	CLA	C1-C2-C3	2.57	130.49	126.04
18	2	610	CLA	CMA-C3A-C2A	-2.57	110.10	116.10
20	1	616	XAT	O24-C25-C24	-2.57	111.45	113.38
18	3	604	CLA	CHD-C1D-ND	-2.56	122.10	124.45
17	4	615	CHL	OMC-CMC-C2C	-2.56	120.92	125.03
18	A	813	CLA	C1-C2-C3	2.56	130.47	126.04
18	B	819	CLA	CHD-C1D-ND	-2.56	122.10	124.45
18	3	603	CLA	C1-C2-C3	2.56	130.46	126.04
18	1	603	CLA	C1-C2-C3	2.55	130.46	126.04
18	A	803	CLA	CHB-C1B-NB	2.55	126.96	124.26
18	B	826	CLA	C1-C2-C3	2.55	130.45	126.04
18	A	843	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
19	4	616	LUT	C35-C15-C14	2.54	128.68	123.47
17	4	607	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
18	A	828	CLA	CHB-C1B-NB	2.54	126.94	124.26
17	2	605	CHL	O1D-CGD-CBD	-2.54	120.52	124.74
18	2	602	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
18	4	609	CLA	C1-C2-C3	2.53	130.42	126.04
17	2	607	CHL	C1A-CHA-C4D	2.53	123.20	118.98
18	B	806	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
18	A	809	CLA	C1-C2-C3	2.53	130.42	126.04
17	2	606	CHL	CHA-C1A-C2A	-2.53	127.37	133.31
18	A	834	CLA	C1-C2-C3	2.53	130.42	126.04
17	2	605	CHL	CHA-C1A-C2A	-2.53	127.37	133.31
19	2	615	LUT	C39-C29-C28	2.53	122.06	118.08
18	A	829	CLA	C1-C2-C3	2.53	130.41	126.04
18	A	840	CLA	C1-C2-C3	2.53	130.41	126.04
18	A	818	CLA	C1-C2-C3	2.52	130.40	126.04
18	B	807	CLA	CHD-C1D-ND	-2.52	122.14	124.45
18	K	201	CLA	CMA-C3A-C2A	-2.52	110.22	116.10
17	2	607	CHL	CHA-C1A-C2A	-2.52	127.40	133.31
18	B	826	CLA	CHD-C1D-ND	-2.51	122.14	124.45
18	A	838	CLA	C1-C2-C3	2.51	130.39	126.04
18	A	805	CLA	O2A-CGA-CBA	2.51	122.10	114.03
18	3	604	CLA	CHB-C1B-NB	2.51	126.92	124.26
18	A	821	CLA	C1-C2-C3	2.51	130.38	126.04
18	B	839	CLA	C1-C2-C3	2.50	130.37	126.04
18	B	831	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
19	2	615	LUT	C32-C33-C34	2.50	122.78	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	806	CLA	C1-C2-C3	2.50	130.37	126.04
17	4	607	CHL	C1A-CHA-C4D	2.50	123.15	118.98
18	H	201	CLA	C1-C2-C3	2.49	130.36	126.04
18	B	825	CLA	C1-C2-C3	2.49	130.35	126.04
18	B	840	CLA	CHB-C1B-NB	2.49	126.90	124.26
17	2	607	CHL	OMC-CMC-C2C	-2.49	121.04	125.03
18	1	614	CLA	CHD-C1D-ND	-2.49	122.17	124.45
18	A	830	CLA	C12-C11-C10	-2.49	101.81	113.24
18	A	829	CLA	C12-C11-C10	-2.49	101.81	113.24
18	A	803	CLA	C1-C2-C3	2.49	130.34	126.04
18	A	839	CLA	C1-C2-C3	2.48	130.77	126.75
18	A	802	CLA	C12-C11-C10	-2.48	101.82	113.24
18	B	818	CLA	CHB-C1B-NB	2.48	126.89	124.26
18	A	823	CLA	CHB-C1B-NB	2.48	126.88	124.26
18	B	812	CLA	C1-C2-C3	2.48	130.33	126.04
18	A	829	CLA	CHB-C1B-NB	2.47	126.88	124.26
18	A	842	CLA	C1-C2-C3	2.47	130.32	126.04
19	4	616	LUT	C39-C29-C28	2.47	121.97	118.08
18	B	835	CLA	CHB-C1B-NB	2.47	126.88	124.26
18	B	805	CLA	C5-C3-C2	2.47	126.12	121.12
18	2	603	CLA	CHB-C1B-NB	2.47	126.87	124.26
18	1	608	CLA	C1-C2-C3	2.47	130.31	126.04
18	B	831	CLA	C1-C2-C3	2.47	130.31	126.04
18	A	802	CLA	C1-C2-C3	2.47	130.31	126.04
17	1	601	CHL	OMC-CMC-C2C	-2.47	121.08	125.03
18	B	832	CLA	C3C-C4C-NC	-2.46	107.81	110.57
18	A	816	CLA	CHD-C1D-ND	-2.46	122.19	124.45
18	B	824	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
18	4	601	CLA	O2A-CGA-CBA	2.46	121.94	112.23
18	B	810	CLA	C1-C2-C3	2.46	130.29	126.04
20	2	616	XAT	C27-C28-C29	2.45	129.33	125.53
18	A	814	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
18	1	611	CLA	O2A-CGA-CBA	2.45	121.89	114.03
18	4	604	CLA	CHB-C1B-NB	2.45	126.85	124.26
18	4	602	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
20	3	615	XAT	C7-C8-C9	2.44	129.32	125.53
18	A	828	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
18	3	603	CLA	C4-C3-C5	-2.44	111.17	115.27
18	A	810	CLA	C3C-C4C-NC	-2.44	107.84	110.57
18	A	843	CLA	O2A-CGA-O1A	-2.44	117.45	123.59
18	B	827	CLA	CHB-C1B-NB	2.43	126.83	124.26
18	B	833	CLA	C12-C11-C10	-2.43	102.06	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	820	CLA	O1D-CGD-CBD	-2.43	119.51	124.48
18	B	808	CLA	C1-C2-C3	2.43	130.24	126.04
18	A	802	CLA	C3C-C4C-NC	-2.43	107.85	110.57
18	B	828	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
17	4	607	CHL	O1D-CGD-CBD	-2.42	120.70	124.74
18	L	303	CLA	C3C-C4C-NC	-2.42	107.85	110.57
18	4	602	CLA	O1D-CGD-CBD	-2.42	119.53	124.48
17	3	616	CHL	C1A-CHA-C4D	2.42	123.02	118.98
18	4	604	CLA	O2A-CGA-CBA	2.42	121.81	114.03
17	2	606	CHL	O1D-CGD-CBD	-2.42	120.71	124.74
18	A	826	CLA	C1-C2-C3	2.42	130.22	126.04
18	B	830	CLA	CHB-C1B-NB	2.41	126.81	124.26
18	B	835	CLA	C1-C2-C3	2.41	130.66	126.75
18	A	811	CLA	C12-C11-C10	-2.41	102.16	113.24
18	A	836	CLA	O2A-CGA-CBA	2.41	121.78	114.03
18	4	614	CLA	C1-C2-C3	2.41	130.65	126.75
18	1	609	CLA	CHB-C1B-NB	2.41	126.81	124.26
18	2	602	CLA	C12-C11-C10	-2.41	102.16	113.24
18	A	827	CLA	C4-C3-C5	-2.41	111.22	115.27
17	4	606	CHL	CBC-CAC-C3C	-2.41	109.35	112.88
18	3	602	CLA	C12-C11-C10	-2.41	102.17	113.24
18	4	602	CLA	CHB-C1B-NB	2.41	126.81	124.26
18	3	609	CLA	CAA-C2A-C3A	-2.41	110.48	116.10
17	2	614	CHL	OMC-CMC-C2C	-2.41	121.18	125.03
18	1	605	CLA	CHB-C1B-NB	2.40	126.80	124.26
18	A	825	CLA	C12-C11-C10	-2.40	102.19	113.24
18	L	302	CLA	O2A-CGA-CBA	2.40	121.75	114.03
18	A	833	CLA	C12-C11-C10	-2.40	102.20	113.24
18	A	806	CLA	C12-C11-C10	-2.40	102.20	113.24
18	A	826	CLA	C12-C11-C10	-2.40	102.20	113.24
18	2	611	CLA	O2A-CGA-CBA	2.40	121.74	114.03
18	B	817	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
18	B	816	CLA	C1-C2-C3	2.40	130.19	126.04
18	4	602	CLA	C12-C11-C10	-2.40	102.23	113.24
18	2	613	CLA	CHB-C1B-NB	2.40	126.79	124.26
18	4	603	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
21	A	850	BCR	C7-C8-C9	-2.39	122.62	126.23
18	2	613	CLA	O1D-CGD-CBD	-2.39	119.59	124.48
18	B	819	CLA	C1-C2-C3	2.39	130.62	126.75
18	B	822	CLA	C3C-C4C-NC	-2.39	107.89	110.57
18	1	608	CLA	C12-C11-C10	-2.39	102.28	113.24
18	A	825	CLA	C1-C2-C3	2.39	130.17	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	614	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
18	B	837	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
17	4	605	CHL	O1D-CGD-CBD	-2.38	120.77	124.74
18	B	815	CLA	C1-C2-C3	2.38	130.16	126.04
18	B	823	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
18	A	841	CLA	C1-C2-C3	2.38	130.16	126.04
18	1	608	CLA	C4-C3-C5	-2.38	111.27	115.27
18	1	602	CLA	CHB-C1B-NB	2.38	126.78	124.26
17	2	601	CHL	OMC-CMC-C2C	-2.38	121.22	125.03
18	A	821	CLA	C12-C11-C10	-2.38	102.32	113.24
18	1	603	CLA	CHB-C1B-NB	2.38	126.77	124.26
18	A	842	CLA	C12-C11-C10	-2.37	102.33	113.24
18	4	614	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
18	A	824	CLA	C1-C2-C3	2.37	130.15	126.04
18	B	823	CLA	C12-C11-C10	-2.37	102.34	113.24
18	A	829	CLA	O2A-CGA-O1A	-2.37	117.61	123.59
19	1	619	LUT	C32-C33-C34	2.37	122.58	118.94
18	B	838	CLA	C12-C11-C10	-2.37	102.36	113.24
18	3	602	CLA	C1-C2-C3	2.36	130.13	126.04
18	3	611	CLA	O2A-CGA-CBA	2.36	121.63	114.03
21	A	846	BCR	C21-C20-C19	2.36	130.59	123.22
18	A	804	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
18	B	833	CLA	C3C-C4C-NC	-2.36	107.92	110.57
18	B	813	CLA	C4-C3-C5	-2.36	111.30	115.27
18	B	816	CLA	C3C-C4C-NC	-2.36	107.92	110.57
18	L	303	CLA	C12-C11-C10	-2.36	102.40	113.24
18	B	806	CLA	C1-C2-C3	2.36	130.12	126.04
17	4	606	CHL	OMC-CMC-C2C	-2.36	121.25	125.03
18	B	814	CLA	C1-C2-C3	2.36	130.12	126.04
18	K	203	CLA	O2A-CGA-CBA	2.36	121.54	112.23
18	3	602	CLA	C4-C3-C5	-2.35	111.31	115.27
18	A	834	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
18	G	204	CLA	CHB-C1B-NB	2.35	126.75	124.26
18	A	821	CLA	CHB-C1B-NB	2.35	126.74	124.26
18	B	809	CLA	C3C-C4C-NC	-2.35	107.94	110.57
18	A	834	CLA	C12-C11-C10	-2.35	102.45	113.24
18	B	818	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
18	K	202	CLA	O2A-CGA-CBA	2.34	121.56	114.03
18	B	820	CLA	C4-C3-C5	-2.34	111.33	115.27
18	B	824	CLA	C1-C2-C3	2.34	130.54	126.75
18	B	832	CLA	O2A-CGA-CBA	2.34	121.56	114.03
18	A	834	CLA	CHB-C1B-NB	2.34	126.73	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	204	CLA	O2A-CGA-CBA	2.34	121.55	114.03
18	F	304	CLA	CAA-C2A-C3A	-2.34	110.64	116.10
18	A	812	CLA	C4-C3-C5	-2.34	111.34	115.27
18	A	840	CLA	C12-C11-C10	-2.34	102.49	113.24
18	A	824	CLA	C3C-C4C-NC	-2.34	107.95	110.57
19	1	615	LUT	C39-C29-C28	2.34	121.76	118.08
18	A	843	CLA	O1D-CGD-CBD	-2.34	119.70	124.48
18	A	819	CLA	C12-C11-C10	-2.34	102.50	113.24
18	A	843	CLA	C1-C2-C3	2.34	130.08	126.04
18	B	816	CLA	CHB-C1B-NB	2.34	126.73	124.26
18	3	607	CLA	O2A-CGA-CBA	2.33	121.52	114.03
18	K	201	CLA	OBD-CAD-CBD	-2.33	121.21	125.97
18	B	805	CLA	CHB-C1B-NB	2.33	126.73	124.26
18	3	609	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
18	A	817	CLA	C12-C11-C10	-2.33	102.53	113.24
19	1	619	LUT	C8-C9-C10	2.33	122.52	118.94
18	4	610	CLA	C12-C11-C10	-2.33	102.54	113.24
18	2	603	CLA	O2A-CGA-CBA	2.33	121.50	114.03
18	2	603	CLA	C3C-C4C-NC	-2.32	107.97	110.57
18	1	612	CLA	C1-C2-C3	2.32	130.06	126.04
18	A	808	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
18	B	822	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
18	B	839	CLA	C12-C11-C10	-2.32	102.58	113.24
19	2	615	LUT	C12-C13-C14	2.32	122.50	118.94
19	3	614	LUT	C12-C13-C14	2.32	122.50	118.94
18	A	826	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	B	821	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	J	102	CLA	CHB-C1B-NB	2.32	126.71	124.26
18	1	609	CLA	C12-C11-C10	-2.32	102.59	113.24
17	4	606	CHL	O1D-CGD-CBD	-2.32	120.88	124.74
18	3	604	CLA	O2A-CGA-CBA	2.32	121.48	114.03
18	B	812	CLA	C4-C3-C5	-2.32	111.37	115.27
18	4	613	CLA	O2A-CGA-CBA	2.32	121.47	114.03
18	B	817	CLA	C3C-C4C-NC	-2.31	107.97	110.57
18	A	824	CLA	O1D-CGD-CBD	-2.31	119.75	124.48
17	4	615	CHL	CHA-C1A-C2A	-2.31	127.87	133.31
18	B	823	CLA	C4-C3-C5	-2.31	111.38	115.27
17	3	616	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
18	B	807	CLA	C4-C3-C5	-2.31	111.38	115.27
18	B	806	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	B	830	CLA	C3C-C4C-NC	-2.31	107.98	110.57
18	B	822	CLA	C1-C2-C3	2.31	130.04	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	841	CLA	C12-C11-C10	-2.31	102.63	113.24
18	A	843	CLA	C12-C11-C10	-2.31	102.64	113.24
18	A	840	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
18	3	602	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	B	826	CLA	CHB-C1B-NB	2.31	126.70	124.26
18	B	818	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
18	4	612	CLA	C4-C3-C5	-2.30	111.40	115.27
18	1	613	CLA	O1D-CGD-CBD	-2.30	119.77	124.48
18	3	608	CLA	O2A-CGA-CBA	2.30	121.43	114.03
18	B	809	CLA	C1-C2-C3	2.30	130.02	126.04
18	A	819	CLA	C4-C3-C5	-2.30	111.40	115.27
18	A	806	CLA	C3C-C4C-NC	-2.30	107.99	110.57
18	A	831	CLA	C1-C2-C3	2.30	130.47	126.75
20	2	616	XAT	O24-C25-C24	-2.30	111.66	113.38
18	A	820	CLA	O2A-CGA-CBA	2.30	121.42	114.03
18	K	202	CLA	CHB-C1B-NB	2.30	126.69	124.26
18	A	813	CLA	C4-C3-C5	-2.30	111.41	115.27
18	A	824	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
18	B	829	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
19	4	616	LUT	C19-C9-C8	2.30	121.69	118.08
18	B	826	CLA	C12-C11-C10	-2.29	102.69	113.24
18	1	603	CLA	C3C-C4C-NC	-2.29	108.00	110.57
18	4	608	CLA	O2A-CGA-CBA	2.29	121.40	114.03
18	K	201	CLA	CHB-C1B-NB	2.29	126.69	124.26
18	L	303	CLA	C4-C3-C5	-2.29	111.41	115.27
17	1	606	CHL	CBC-CAC-C3C	-2.29	109.52	112.88
17	1	606	CHL	OMC-CMC-C2C	-2.29	121.36	125.03
18	B	805	CLA	C12-C11-C10	-2.29	102.71	113.24
18	3	606	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	K	203	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
18	1	612	CLA	C4-C3-C5	-2.29	111.42	115.27
18	A	818	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	B	837	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
18	3	603	CLA	CHB-C1B-NB	2.29	126.68	124.26
18	B	831	CLA	C12-C11-C10	-2.29	102.73	113.24
18	4	614	CLA	CHB-C1B-NB	2.28	126.67	124.26
18	1	613	CLA	O2A-CGA-CBA	2.28	121.36	114.03
18	3	617	CLA	CHB-C1B-NB	2.28	126.67	124.26
18	A	832	CLA	C3C-C4C-NC	-2.28	108.02	110.57
18	A	808	CLA	C1-C2-C3	2.28	130.43	126.75
18	A	817	CLA	C3C-C4C-NC	-2.27	108.02	110.57
17	4	605	CHL	O2A-CGA-O1A	-2.27	117.86	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	802	CLA	C2C-C1C-NC	-2.27	107.84	109.97
18	A	827	CLA	C12-C11-C10	-2.27	102.80	113.24
18	2	604	CLA	C12-C11-C10	-2.27	102.80	113.24
18	B	820	CLA	C3C-C4C-NC	-2.27	108.02	110.57
18	1	604	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	3	610	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	3	612	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	B	802	CLA	C4-C3-C5	-2.27	111.45	115.27
18	A	818	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	B	804	CLA	C12-C11-C10	-2.27	102.81	113.24
18	A	819	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	A	819	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
18	4	610	CLA	C1-C2-C3	2.27	129.97	126.04
18	A	835	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	4	602	CLA	C3C-C4C-NC	-2.27	108.03	110.57
18	F	303	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	A	803	CLA	C12-C11-C10	-2.27	102.83	113.24
18	A	825	CLA	CHB-C1B-NB	2.27	126.66	124.26
18	B	838	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
18	2	602	CLA	C3C-C4C-NC	-2.26	108.03	110.57
20	3	615	XAT	C27-C28-C29	2.26	129.04	125.53
18	A	837	CLA	C1-C2-C3	2.26	129.95	126.04
18	B	840	CLA	C3C-C4C-NC	-2.26	108.04	110.57
18	B	827	CLA	C12-C11-C10	-2.26	102.86	113.24
18	1	612	CLA	C12-C11-C10	-2.26	102.88	113.24
18	4	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
18	B	817	CLA	C12-C11-C10	-2.25	102.88	113.24
18	H	201	CLA	C3C-C4C-NC	-2.25	108.04	110.57
18	1	610	CLA	CHB-C1B-NB	2.25	126.64	124.26
18	A	808	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	B	836	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	B	822	CLA	C12-C11-C10	-2.25	102.90	113.24
18	4	603	CLA	C2D-C1D-ND	2.25	111.76	110.10
18	B	813	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	1	607	CLA	O2A-CGA-CBA	2.25	121.25	114.03
18	A	804	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
17	2	607	CHL	O2A-CGA-O1A	-2.25	117.92	123.59
18	A	815	CLA	CHB-C1B-NB	2.25	126.63	124.26
18	A	821	CLA	C3C-C4C-NC	-2.25	108.05	110.57
18	A	838	CLA	C3C-C4C-NC	-2.24	108.05	110.57
18	B	803	CLA	C3C-C4C-NC	-2.24	108.06	110.57
18	B	811	CLA	C3C-C4C-NC	-2.24	108.06	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	L	304	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	4	609	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	B	804	CLA	O2A-CGA-O1A	-2.24	117.93	123.59
18	A	810	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
18	4	610	CLA	CHB-C1B-NB	2.24	126.63	124.26
18	A	810	CLA	C1-C2-C3	2.24	130.37	126.75
18	A	830	CLA	C3C-C4C-NC	-2.24	108.06	110.57
18	3	613	CLA	CHB-C1B-NB	2.24	126.63	124.26
19	3	614	LUT	C1-C6-C7	2.24	122.11	115.78
18	B	801	CLA	C12-C11-C10	-2.24	102.96	113.24
18	B	836	CLA	O2D-CGD-O1D	-2.24	119.47	123.84
18	1	611	CLA	CHB-C1B-NB	2.23	126.62	124.26
18	2	602	CLA	CHB-C1B-NB	2.23	126.62	124.26
18	B	809	CLA	C12-C11-C10	-2.23	102.97	113.24
17	2	614	CHL	CHA-C1A-C2A	-2.23	128.06	133.31
18	2	612	CLA	O1D-CGD-CBD	-2.23	119.92	124.48
18	G	203	CLA	CHB-C1B-NB	2.23	126.62	124.26
18	1	602	CLA	C12-C11-C10	-2.23	102.99	113.24
18	A	814	CLA	O2A-CGA-CBA	2.23	121.19	114.03
18	B	836	CLA	C12-C11-C10	-2.23	103.00	113.24
18	2	608	CLA	CHB-C1B-NB	2.23	126.62	124.26
18	A	831	CLA	CHB-C1B-NB	2.23	126.61	124.26
18	1	609	CLA	C3C-C4C-NC	-2.22	108.14	110.57
18	F	301	CLA	C12-C11-C10	-2.22	102.55	113.29
18	B	824	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	B	812	CLA	C11-C12-C13	2.22	123.10	115.92
18	2	611	CLA	CHB-C1B-NB	2.22	126.61	124.26
18	A	839	CLA	CHB-C1B-NB	2.22	126.61	124.26
18	B	837	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
17	4	605	CHL	OMC-CMC-C2C	-2.22	121.47	125.03
18	B	840	CLA	C1-C2-C3	2.22	129.89	126.04
18	B	802	CLA	C12-C11-C10	-2.22	103.03	113.24
18	A	822	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	A	807	CLA	C12-C11-C10	-2.22	103.04	113.24
18	B	836	CLA	CHB-C1B-NB	2.22	126.61	124.26
18	1	614	CLA	O2A-CGA-CBA	2.22	121.16	114.03
18	B	829	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	A	814	CLA	O2D-CGD-O1D	-2.22	119.50	123.84
18	2	612	CLA	C3C-C4C-NC	-2.22	108.08	110.57
18	A	820	CLA	CHB-C1B-NB	2.22	126.60	124.26
18	B	807	CLA	C12-C11-C10	-2.22	103.06	113.24
18	A	842	CLA	CHB-C1B-NB	2.22	126.60	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	803	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	B	812	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	A	807	CLA	CHB-C1B-NB	2.21	126.60	124.26
18	2	608	CLA	O2A-CGA-CBA	2.21	121.14	114.03
21	2	618	BCR	C10-C11-C12	2.21	130.12	123.22
18	B	801	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	A	812	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	G	203	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	A	804	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
18	2	612	CLA	C1-C2-C3	2.21	129.86	126.04
18	B	805	CLA	C3C-C4C-NC	-2.21	108.09	110.57
18	B	810	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	B	828	CLA	C3C-C4C-NC	-2.21	108.10	110.57
18	3	613	CLA	CAA-C2A-C3A	-2.20	110.95	116.10
18	2	604	CLA	CHB-C1B-NB	2.20	126.59	124.26
18	B	807	CLA	CHB-C1B-NB	2.20	126.59	124.26
17	4	607	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
18	1	602	CLA	C3C-C4C-NC	-2.20	108.10	110.57
18	B	832	CLA	CMD-C2D-C1D	2.20	128.59	124.71
18	3	602	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
18	B	804	CLA	C3C-C4C-NC	-2.20	108.10	110.57
17	2	606	CHL	OMC-CMC-C2C	-2.20	121.50	125.03
18	B	815	CLA	CHB-C1B-NB	2.20	126.59	124.26
18	B	839	CLA	C3C-C4C-NC	-2.20	108.10	110.57
18	2	611	CLA	O1D-CGD-CBD	-2.20	119.98	124.48
18	A	813	CLA	C12-C11-C10	-2.20	103.14	113.24
18	A	843	CLA	CHB-C1B-NB	2.20	126.58	124.26
18	A	826	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
18	L	302	CLA	CHB-C1B-NB	2.19	126.58	124.26
17	2	601	CHL	O2A-CGA-CBA	2.19	120.90	112.23
18	B	808	CLA	C3C-C4C-NC	-2.19	108.11	110.57
18	2	612	CLA	C4-C3-C5	-2.19	111.58	115.27
18	A	826	CLA	C3C-C4C-NC	-2.19	108.11	110.57
18	3	607	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
19	1	615	LUT	C12-C13-C14	2.19	122.30	118.94
18	B	817	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
18	1	612	CLA	CHB-C1B-NB	2.19	126.58	124.26
18	B	824	CLA	CHB-C1B-NB	2.19	126.58	124.26
18	A	807	CLA	C5-C3-C2	2.19	125.55	121.12
18	1	613	CLA	O2D-CGD-O1D	-2.19	119.56	123.84
18	B	828	CLA	C1-C2-C3	2.19	129.83	126.04
18	B	813	CLA	C12-C11-C10	-2.19	103.19	113.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	803	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
18	4	603	CLA	CHB-C1B-NB	2.19	126.57	124.26
18	A	835	CLA	O2A-CGA-CBA	2.19	121.06	114.03
18	B	831	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
18	B	829	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
18	A	808	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	A	819	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
18	A	835	CLA	O1D-CGD-CBD	-2.18	120.01	124.48
18	A	841	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	1	605	CLA	C2A-C1A-CHA	2.18	126.10	122.71
18	2	610	CLA	CHB-C1B-NB	2.18	126.57	124.26
18	3	610	CLA	C2D-C1D-ND	2.18	111.71	110.10
18	B	817	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
18	A	812	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	A	831	CLA	C3C-C4C-NC	-2.18	108.13	110.57
18	B	811	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	B	823	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
18	4	613	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	2	604	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
18	A	807	CLA	C3C-C4C-NC	-2.18	108.13	110.57
18	A	824	CLA	CHB-C1B-NB	2.18	126.56	124.26
18	1	603	CLA	O1D-CGD-CBD	-2.17	120.04	124.48
18	1	607	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	A	828	CLA	C12-C11-C10	-2.17	103.26	113.24
18	B	832	CLA	C2C-C1C-NC	-2.17	107.94	109.97
18	L	304	CLA	CED-O2D-CGD	2.17	120.85	115.94
18	B	823	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	B	822	CLA	CED-O2D-CGD	2.17	120.85	115.94
18	B	823	CLA	C2D-C1D-ND	2.17	111.70	110.10
18	A	854	CLA	CHB-C1B-NB	2.17	126.56	124.26
18	3	602	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
18	B	838	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	A	836	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	2	610	CLA	CAA-C2A-C3A	-2.17	111.04	116.10
18	B	802	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
18	A	814	CLA	CHB-C1B-NB	2.17	126.55	124.26
18	K	203	CLA	CHB-C1B-NB	2.17	126.55	124.26
18	G	202	CLA	O2A-CGA-CBA	2.17	120.99	114.03
18	A	811	CLA	C2D-C1D-ND	2.17	111.70	110.10
18	B	820	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
18	K	203	CLA	C3C-C4C-NC	-2.17	108.14	110.57
18	A	812	CLA	O2D-CGD-O1D	-2.17	119.61	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	833	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	A	840	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	1	603	CLA	CMD-C2D-C1D	2.16	128.53	124.71
18	B	819	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
18	F	303	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	1	604	CLA	C3C-C4C-NC	-2.16	108.14	110.57
18	H	201	CLA	CHB-C1B-NB	2.16	126.55	124.26
18	4	601	CLA	C3C-C4C-NC	-2.16	108.15	110.57
18	A	812	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
18	3	607	CLA	CHB-C1B-NB	2.16	126.54	124.26
18	4	611	CLA	CHB-C1B-NB	2.16	126.54	124.26
18	3	603	CLA	O1D-CGD-CBD	-2.16	120.07	124.48
18	4	612	CLA	C1-C2-C3	2.15	129.77	126.04
18	A	825	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	B	806	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	B	814	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
18	3	611	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	1	608	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	3	612	CLA	CAA-C2A-C3A	-2.15	111.07	116.10
18	A	811	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	H	201	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	B	840	CLA	C4-C3-C5	-2.15	111.66	115.27
18	A	820	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	3	608	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	3	617	CLA	C3C-C4C-NC	-2.15	108.16	110.57
18	A	817	CLA	C5-C3-C2	2.15	125.46	121.12
18	B	823	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	1	602	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
18	A	804	CLA	C3C-C4C-NC	-2.15	108.17	110.57
18	A	841	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	841	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
18	B	826	CLA	C4-C3-C5	-2.14	111.67	115.27
18	B	814	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
17	2	605	CHL	OMC-CMC-C2C	-2.14	121.60	125.03
18	B	824	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
18	B	827	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	814	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	819	CLA	O1D-CGD-CBD	-2.14	120.11	124.48
18	2	610	CLA	C2D-C1D-ND	2.14	111.68	110.10
18	B	822	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
18	A	839	CLA	C3C-C4C-NC	-2.14	108.17	110.57
18	A	832	CLA	CHB-C1B-NB	2.14	126.52	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	F	304	CLA	CHB-C1B-NB	2.14	126.52	124.26
18	A	815	CLA	C3C-C4C-NC	-2.14	108.18	110.57
18	2	604	CLA	C4-C3-C5	-2.14	111.68	115.27
18	B	806	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	A	830	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
18	2	612	CLA	O2D-CGD-O1D	-2.13	119.67	123.84
18	3	613	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	3	611	CLA	CHB-C1B-NB	2.13	126.52	124.26
18	3	603	CLA	CMD-C2D-C1D	2.13	128.47	124.71
18	1	607	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	B	834	CLA	CMD-C2D-C1D	2.13	128.47	124.71
18	A	829	CLA	C3C-C4C-NC	-2.13	108.18	110.57
18	1	614	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	B	827	CLA	C4-C3-C5	-2.13	111.69	115.27
18	B	831	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	B	831	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
18	G	202	CLA	C3C-C4C-NC	-2.13	108.19	110.57
18	A	811	CLA	CHB-C1B-NB	2.13	126.51	124.26
18	L	304	CLA	O1D-CGD-CBD	-2.12	120.14	124.48
18	2	602	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
18	B	826	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
18	B	827	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
18	B	815	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	3	609	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	B	825	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	A	833	CLA	C4-C3-C5	-2.12	111.70	115.27
18	2	604	CLA	C3C-C4C-NC	-2.12	108.19	110.57
18	A	804	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	2	603	CLA	CMD-C2D-C1D	2.12	128.45	124.71
18	2	612	CLA	CHB-C1B-NB	2.12	126.50	124.26
18	L	304	CLA	O2A-CGA-CBA	2.12	120.84	114.03
18	2	613	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
18	J	102	CLA	CED-O2D-CGD	2.12	120.73	115.94
18	4	604	CLA	C3C-C4C-NC	-2.12	108.20	110.57
18	B	818	CLA	C3C-C4C-NC	-2.12	108.20	110.57
18	B	812	CLA	O2D-CGD-O1D	-2.12	119.70	123.84
18	K	201	CLA	CAA-C2A-C3A	-2.12	111.16	116.10
18	3	617	CLA	C1-C2-C3	2.12	129.70	126.04
18	B	819	CLA	O1D-CGD-CBD	-2.12	120.16	124.48
18	1	613	CLA	CHB-C1B-NB	2.11	126.50	124.26
18	A	808	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	1	612	CLA	C3C-C4C-NC	-2.11	108.20	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	822	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	818	CLA	CMD-C2D-C1D	2.11	128.44	124.71
18	A	807	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
18	4	609	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	A	805	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	A	825	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	B	814	CLA	C3C-C4C-NC	-2.11	108.20	110.57
18	4	612	CLA	C12-C11-C10	-2.11	103.10	113.29
18	A	816	CLA	O2A-CGA-CBA	2.11	120.81	114.03
18	A	854	CLA	CAC-C3C-C2C	2.11	131.14	127.53
17	4	606	CHL	O2A-CGA-O1A	-2.11	118.04	123.30
18	B	838	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
18	B	822	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	802	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	A	854	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
18	B	826	CLA	C3C-C4C-NC	-2.11	108.21	110.57
18	A	810	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
18	L	302	CLA	C3C-C4C-NC	-2.11	108.21	110.57
18	B	837	CLA	CHB-C1B-NB	2.11	126.49	124.26
18	A	822	CLA	O1D-CGD-CBD	-2.11	120.18	124.48
18	K	202	CLA	C3C-C4C-NC	-2.10	108.21	110.57
18	A	832	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
18	B	801	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	A	809	CLA	C3C-C4C-NC	-2.10	108.21	110.57
18	A	836	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
18	B	802	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
18	3	605	CLA	CHB-C1B-NB	2.10	126.48	124.26
18	4	612	CLA	C3C-C4C-NC	-2.10	108.21	110.57
18	B	822	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
18	B	825	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
18	A	804	CLA	C4-C3-C5	-2.10	111.74	115.27
17	3	616	CHL	OMC-CMC-C2C	-2.10	121.67	125.03
18	3	604	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	1	610	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	A	821	CLA	CED-O2D-CGD	2.10	120.68	115.94
18	F	303	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
18	B	804	CLA	O2D-CGD-O1D	-2.10	119.74	123.84
18	1	613	CLA	C3C-C4C-NC	-2.10	108.22	110.57
18	B	825	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
18	B	801	CLA	C4-C3-C5	-2.09	111.75	115.27
18	B	808	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
18	A	839	CLA	O2A-CGA-O1A	-2.09	118.31	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	4	602	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
18	3	611	CLA	CMD-C2D-C1D	2.09	128.40	124.71
19	1	619	LUT	C31-C30-C29	2.09	130.29	127.31
18	2	612	CLA	CMD-C2D-C1D	2.09	128.40	124.71
18	B	828	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
18	A	823	CLA	CAA-C2A-C3A	-2.09	111.22	116.10
18	B	802	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	1	613	CLA	CMD-C2D-C1D	2.09	128.39	124.71
18	4	614	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	2	604	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
18	3	605	CLA	CED-O2D-CGD	2.09	120.66	115.94
18	A	811	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	B	821	CLA	C3C-C4C-NC	-2.09	108.23	110.57
18	A	831	CLA	O1D-CGD-CBD	-2.08	120.22	124.48
18	A	835	CLA	CHB-C1B-NB	2.08	126.46	124.26
18	3	605	CLA	C3C-C4C-NC	-2.08	108.23	110.57
18	A	825	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
18	A	801	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
18	J	102	CLA	CMD-C2D-C1D	2.08	128.38	124.71
18	2	609	CLA	C3C-C4C-NC	-2.08	108.24	110.57
18	A	803	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
18	3	609	CLA	CHB-C1B-NB	2.08	126.46	124.26
17	3	616	CHL	O2A-CGA-CBA	2.08	120.45	112.23
18	A	832	CLA	C5-C3-C2	2.08	125.32	121.12
18	4	609	CLA	C2C-C1C-NC	-2.08	108.03	109.97
18	2	608	CLA	C3C-C4C-NC	-2.07	108.24	110.57
18	2	611	CLA	C2D-C1D-ND	2.07	111.63	110.10
18	A	801	CLA	C12-C11-C10	-2.07	103.71	113.24
18	3	607	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	A	833	CLA	C1-C2-C3	2.07	129.63	126.04
20	4	617	XAT	O4-C5-C4	-2.07	111.82	113.38
18	B	820	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	B	818	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
18	B	838	CLA	CHB-C1B-NB	2.07	126.45	124.26
18	B	811	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	L	303	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
18	A	811	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
18	1	611	CLA	C2D-C1D-ND	2.07	111.63	110.10
18	3	604	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	B	807	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
18	3	617	CLA	C4-C3-C5	-2.07	111.79	115.27
18	2	613	CLA	C3C-C4C-NC	-2.07	108.25	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	G	202	CLA	CHB-C1B-NB	2.07	126.44	124.26
18	G	204	CLA	C3C-C4C-NC	-2.07	108.25	110.57
18	2	602	CLA	CMD-C2D-C1D	2.07	128.35	124.71
18	A	838	CLA	CHB-C1B-NB	2.07	126.44	124.26
18	4	601	CLA	CMD-C2D-C1D	2.06	128.35	124.71
18	A	826	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
18	3	605	CLA	C2D-C1D-ND	2.06	111.62	110.10
18	A	826	CLA	C2C-C1C-NC	-2.06	108.04	109.97
18	B	812	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	A	813	CLA	CHB-C1B-NB	2.06	126.44	124.26
18	A	802	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
18	H	201	CLA	CMD-C2D-C1D	2.06	128.34	124.71
18	3	617	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
18	3	602	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	A	803	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	835	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	810	CLA	CMD-C2D-C1D	2.06	128.34	124.71
18	A	801	CLA	C3C-C4C-NC	-2.06	108.26	110.57
18	B	812	CLA	O1D-CGD-CBD	-2.06	120.28	124.48
21	A	846	BCR	C20-C19-C18	2.06	132.19	126.42
18	A	817	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
18	A	801	CLA	C2D-C1D-ND	2.05	111.62	110.10
18	A	837	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	B	834	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
18	B	803	CLA	O2D-CGD-O1D	-2.05	119.82	123.84
18	B	810	CLA	CHB-C1B-NB	2.05	126.43	124.26
18	A	821	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	B	840	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	B	804	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
18	A	832	CLA	C1-C2-C3	2.05	129.59	126.04
18	L	304	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	4	603	CLA	CMD-C2D-C1D	2.05	128.33	124.71
18	A	807	CLA	CED-O2D-CGD	2.05	120.58	115.94
18	4	608	CLA	C3C-C4C-NC	-2.05	108.27	110.57
18	B	807	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
18	A	842	CLA	C3C-C4C-NC	-2.05	108.28	110.57
18	B	831	CLA	C3C-C4C-NC	-2.05	108.28	110.57
18	A	823	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
18	A	808	CLA	CMD-C2D-C1D	2.05	128.32	124.71
18	A	809	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	B	839	CLA	C4D-CHA-C1A	2.04	123.74	121.25
18	A	822	CLA	CED-O2D-CGD	2.04	120.56	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	807	CLA	O2D-CGD-O1D	-2.04	119.84	123.84
18	B	835	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
18	1	610	CLA	C2D-C1D-ND	2.04	111.61	110.10
18	1	612	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
18	A	827	CLA	C3C-C4C-NC	-2.04	108.28	110.57
18	B	817	CLA	CMD-C2D-C1D	2.04	128.31	124.71
18	A	836	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	B	821	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	J	102	CLA	C3C-C4C-NC	-2.04	108.28	110.57
18	B	803	CLA	CAA-C2A-C3A	-2.04	111.33	116.10
18	4	604	CLA	CED-O2D-CGD	2.04	120.55	115.94
18	L	303	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
18	3	605	CLA	CMD-C2D-C1D	2.04	128.31	124.71
18	3	612	CLA	CMD-C2D-C1D	2.04	128.31	124.71
18	A	840	CLA	C4-C3-C5	-2.04	111.84	115.27
18	J	102	CLA	C2D-C1D-ND	2.04	111.61	110.10
18	A	810	CLA	CHB-C1B-NB	2.04	126.42	124.26
18	A	802	CLA	CHB-C1B-NB	2.04	126.42	124.26
19	2	615	LUT	C31-C30-C29	2.04	130.22	127.31
18	3	612	CLA	C3C-C4C-NC	-2.04	108.29	110.57
18	1	607	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
18	A	827	CLA	O2D-CGD-O1D	-2.04	119.86	123.84
18	A	817	CLA	CHB-C1B-NB	2.04	126.41	124.26
18	B	839	CLA	CHB-C1B-NB	2.04	126.41	124.26
18	4	604	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
18	B	835	CLA	CED-O2D-CGD	2.04	120.54	115.94
18	B	834	CLA	CHB-C1B-NB	2.04	126.41	124.26
18	4	601	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
18	B	819	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	4	613	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
18	A	819	CLA	CMD-C2D-C1D	2.03	128.30	124.71
18	B	809	CLA	CHB-C1B-NB	2.03	126.41	124.26
18	A	807	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
18	3	610	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	A	813	CLA	C3C-C4C-NC	-2.03	108.29	110.57
18	F	301	CLA	C3C-C4C-NC	-2.03	108.29	110.57
17	1	601	CHL	O2A-CGA-O1A	-2.03	118.46	123.59
18	B	837	CLA	CMD-C2D-C1D	2.03	128.29	124.71
17	2	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
18	B	840	CLA	C12-C11-C10	-2.03	103.91	113.24
18	1	614	CLA	C3C-C4C-NC	-2.03	108.30	110.57
18	3	610	CLA	CMD-C2D-C1D	2.03	128.29	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	839	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	A	823	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	3	613	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	3	617	CLA	CMD-C2D-C1D	2.03	128.29	124.71
18	A	827	CLA	CHB-C1B-NB	2.03	126.40	124.26
18	B	804	CLA	CMD-C2D-C1D	2.02	128.28	124.71
18	F	304	CLA	C3C-C4C-NC	-2.02	108.30	110.57
18	L	303	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
18	B	839	CLA	C4-C3-C5	-2.02	111.87	115.27
18	B	817	CLA	C1-C2-C3	2.02	129.54	126.04
18	B	815	CLA	C4-C3-C5	-2.02	111.87	115.27
18	A	825	CLA	CMD-C2D-C1D	2.02	128.27	124.71
18	B	825	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
18	A	805	CLA	CHB-C1B-NB	2.02	126.39	124.26
18	A	810	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
18	4	611	CLA	C3C-C4C-NC	-2.02	108.31	110.57
18	4	613	CLA	C3C-C4C-NC	-2.02	108.31	110.57
18	4	612	CLA	CHB-C1B-NB	2.02	126.39	124.26
18	A	835	CLA	O2D-CGD-O1D	-2.02	119.89	123.84
18	L	302	CLA	O1D-CGD-CBD	-2.02	120.36	124.48
18	A	840	CLA	CED-O2D-CGD	2.02	120.50	115.94
18	1	608	CLA	O2D-CGD-O1D	-2.02	119.90	123.84
18	4	610	CLA	C2D-C1D-ND	2.02	111.59	110.10
18	B	804	CLA	C2D-C1D-ND	2.02	111.59	110.10
19	3	614	LUT	C35-C15-C14	2.01	127.60	123.47
18	B	840	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
18	B	809	CLA	CMD-C2D-C1D	2.01	128.26	124.71
18	3	608	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	A	830	CLA	CHB-C1B-NB	2.01	126.39	124.26
18	F	304	CLA	CED-O2D-CGD	2.01	120.49	115.94
18	3	607	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	F	304	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	A	813	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	4	609	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	1	602	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	1	610	CLA	C3C-C4C-NC	-2.01	108.32	110.57
18	B	821	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
18	B	802	CLA	C2B-C1B-NB	-2.01	108.89	110.23
18	1	602	CLA	CMD-C2D-C1D	2.01	128.25	124.71
18	B	801	CLA	O1D-CGD-CBD	-2.01	120.37	124.48
18	F	301	CLA	C2D-C1D-ND	2.01	111.58	110.10
18	B	819	CLA	CHB-C1B-NB	2.01	126.38	124.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	809	CLA	O2D-CGD-O1D	-2.01	119.91	123.84
18	1	605	CLA	CBD-CHA-C1A	2.01	130.87	128.50
18	A	801	CLA	CHB-C1B-NB	2.01	126.38	124.26
18	K	201	CLA	C3C-C4C-NC	-2.00	108.32	110.57
18	B	826	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
18	1	614	CLA	C2D-C1D-ND	2.00	111.58	110.10
18	A	854	CLA	CMD-C2D-C1D	2.00	128.25	124.71
18	2	611	CLA	C3C-C4C-NC	-2.00	108.33	110.57
18	A	836	CLA	CMD-C2D-C1D	2.00	128.24	124.71
18	A	837	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
18	A	809	CLA	O1D-CGD-CBD	-2.00	120.39	124.48

There are no chirality outliers.

All (1603) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	1	606	CHL	C4C-C3C-CAC-CBC
17	2	601	CHL	CBA-CGA-O2A-C1
17	2	606	CHL	C3A-C2A-CAA-CBA
17	2	607	CHL	C3C-C2C-CMC-OMC
17	2	614	CHL	C1A-C2A-CAA-CBA
17	2	614	CHL	CBD-CGD-O2D-CED
17	3	616	CHL	CBA-CGA-O2A-C1
17	4	605	CHL	C2-C3-C5-C6
17	4	606	CHL	C1A-C2A-CAA-CBA
17	4	607	CHL	C3A-C2A-CAA-CBA
17	4	607	CHL	O2A-C1-C2-C3
17	4	607	CHL	C1-C2-C3-C5
17	4	615	CHL	C1A-C2A-CAA-CBA
18	1	603	CLA	CHA-CBD-CGD-O1D
18	1	608	CLA	C11-C12-C13-C14
18	1	609	CLA	C11-C10-C8-C9
18	1	611	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	C1-C2-C3-C4
18	1	613	CLA	C1A-C2A-CAA-CBA
18	1	613	CLA	C3A-C2A-CAA-CBA
18	2	602	CLA	CBD-CGD-O2D-CED
18	2	603	CLA	CHA-CBD-CGD-O2D
18	2	604	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	C1-C2-C3-C4
18	2	604	CLA	C1-C2-C3-C5
18	2	608	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	2	608	CLA	C3A-C2A-CAA-CBA
18	2	611	CLA	CBD-CGD-O2D-CED
18	2	611	CLA	O1D-CGD-O2D-CED
18	2	612	CLA	C1-C2-C3-C5
18	3	602	CLA	CHA-CBD-CGD-O2D
18	3	603	CLA	C1A-C2A-CAA-CBA
18	3	603	CLA	C3A-C2A-CAA-CBA
18	3	603	CLA	CBD-CGD-O2D-CED
18	3	607	CLA	C1A-C2A-CAA-CBA
18	3	607	CLA	C3A-C2A-CAA-CBA
18	3	610	CLA	CHA-CBD-CGD-O2D
18	3	610	CLA	CBD-CGD-O2D-CED
18	3	612	CLA	C2B-C3B-CAB-CBB
18	3	612	CLA	C4B-C3B-CAB-CBB
18	3	617	CLA	C4-C3-C5-C6
18	4	601	CLA	CHA-CBD-CGD-O1D
18	4	602	CLA	CHA-CBD-CGD-O1D
18	4	608	CLA	C1A-C2A-CAA-CBA
18	4	608	CLA	C3A-C2A-CAA-CBA
18	4	609	CLA	C4-C3-C5-C6
18	4	610	CLA	C1A-C2A-CAA-CBA
18	4	610	CLA	CHA-CBD-CGD-O2D
18	4	611	CLA	C1A-C2A-CAA-CBA
18	4	611	CLA	C3A-C2A-CAA-CBA
18	4	612	CLA	CHA-CBD-CGD-O1D
18	4	612	CLA	CHA-CBD-CGD-O2D
18	4	612	CLA	C1-C2-C3-C4
18	4	612	CLA	C1-C2-C3-C5
18	A	801	CLA	CBD-CGD-O2D-CED
18	A	801	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C2B-C3B-CAB-CBB
18	A	802	CLA	C4B-C3B-CAB-CBB
18	A	804	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	O2A-C1-C2-C3
18	A	805	CLA	C1A-C2A-CAA-CBA
18	A	805	CLA	C3A-C2A-CAA-CBA
18	A	805	CLA	C2B-C3B-CAB-CBB
18	A	805	CLA	C4B-C3B-CAB-CBB
18	A	806	CLA	CHA-CBD-CGD-O1D
18	A	806	CLA	CHA-CBD-CGD-O2D
18	A	806	CLA	CAD-CBD-CGD-O1D
18	A	806	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	CHA-CBD-CGD-O1D
18	A	809	CLA	CHA-CBD-CGD-O2D
18	A	810	CLA	C1A-C2A-CAA-CBA
18	A	810	CLA	C3A-C2A-CAA-CBA
18	A	813	CLA	C2B-C3B-CAB-CBB
18	A	813	CLA	C4B-C3B-CAB-CBB
18	A	815	CLA	C1A-C2A-CAA-CBA
18	A	815	CLA	C3A-C2A-CAA-CBA
18	A	815	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	C1A-C2A-CAA-CBA
18	A	817	CLA	C2-C3-C5-C6
18	A	817	CLA	C4-C3-C5-C6
18	A	819	CLA	C3A-C2A-CAA-CBA
18	A	819	CLA	CHA-CBD-CGD-O2D
18	A	819	CLA	C1-C2-C3-C5
18	A	820	CLA	C2B-C3B-CAB-CBB
18	A	820	CLA	C4B-C3B-CAB-CBB
18	A	821	CLA	CBD-CGD-O2D-CED
18	A	822	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	C3A-C2A-CAA-CBA
18	A	824	CLA	CBD-CGD-O2D-CED
18	A	824	CLA	C2-C3-C5-C6
18	A	825	CLA	O1A-CGA-O2A-C1
18	A	825	CLA	C2B-C3B-CAB-CBB
18	A	825	CLA	C4B-C3B-CAB-CBB
18	A	827	CLA	C2B-C3B-CAB-CBB
18	A	827	CLA	C4B-C3B-CAB-CBB
18	A	827	CLA	C14-C13-C15-C16
18	A	829	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	C11-C10-C8-C7
18	A	829	CLA	C11-C12-C13-C14
18	A	830	CLA	C2B-C3B-CAB-CBB
18	A	830	CLA	C4B-C3B-CAB-CBB
18	A	830	CLA	C2-C3-C5-C6
18	A	830	CLA	C4-C3-C5-C6
18	A	831	CLA	C1A-C2A-CAA-CBA
18	A	831	CLA	CBA-CGA-O2A-C1
18	A	831	CLA	O1A-CGA-O2A-C1
18	A	836	CLA	C1A-C2A-CAA-CBA
18	A	836	CLA	C3A-C2A-CAA-CBA
18	A	836	CLA	CHA-CBD-CGD-O1D
18	A	837	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
18	A	837	CLA	C4B-C3B-CAB-CBB
18	A	837	CLA	C2-C3-C5-C6
18	A	837	CLA	C4-C3-C5-C6
18	A	839	CLA	C1A-C2A-CAA-CBA
18	A	839	CLA	CAD-CBD-CGD-O2D
18	A	839	CLA	C1-C2-C3-C4
18	A	839	CLA	C1-C2-C3-C5
18	A	840	CLA	C2B-C3B-CAB-CBB
18	A	840	CLA	C4B-C3B-CAB-CBB
18	A	840	CLA	CHA-CBD-CGD-O1D
18	A	840	CLA	CHA-CBD-CGD-O2D
18	A	840	CLA	C1-C2-C3-C4
18	A	841	CLA	C2-C3-C5-C6
18	A	841	CLA	C4-C3-C5-C6
18	A	843	CLA	C2B-C3B-CAB-CBB
18	A	843	CLA	C4B-C3B-CAB-CBB
18	B	801	CLA	CHA-CBD-CGD-O1D
18	B	802	CLA	C3A-C2A-CAA-CBA
18	B	802	CLA	C1-C2-C3-C5
18	B	802	CLA	C14-C13-C15-C16
18	B	804	CLA	C3A-C2A-CAA-CBA
18	B	807	CLA	C11-C12-C13-C14
18	B	809	CLA	C1A-C2A-CAA-CBA
18	B	809	CLA	C1-C2-C3-C4
18	B	810	CLA	C1-C2-C3-C4
18	B	812	CLA	C3A-C2A-CAA-CBA
18	B	812	CLA	C2B-C3B-CAB-CBB
18	B	812	CLA	C4B-C3B-CAB-CBB
18	B	813	CLA	C2B-C3B-CAB-CBB
18	B	813	CLA	C4B-C3B-CAB-CBB
18	B	813	CLA	CBD-CGD-O2D-CED
18	B	813	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	C2A-CAA-CBA-CGA
18	B	816	CLA	C1-C2-C3-C4
18	B	816	CLA	C1-C2-C3-C5
18	B	817	CLA	C3A-C2A-CAA-CBA
18	B	817	CLA	C4-C3-C5-C6
18	B	819	CLA	C1A-C2A-CAA-CBA
18	B	820	CLA	CBA-CGA-O2A-C1
18	B	820	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	C1-C2-C3-C4
18	B	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
18	B	821	CLA	C4-C3-C5-C6
18	B	822	CLA	C1A-C2A-CAA-CBA
18	B	822	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	C1-C2-C3-C4
18	B	822	CLA	C1-C2-C3-C5
18	B	823	CLA	C2B-C3B-CAB-CBB
18	B	823	CLA	C4B-C3B-CAB-CBB
18	B	824	CLA	C2B-C3B-CAB-CBB
18	B	824	CLA	C4B-C3B-CAB-CBB
18	B	825	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C3A-C2A-CAA-CBA
18	B	826	CLA	C2B-C3B-CAB-CBB
18	B	826	CLA	C4B-C3B-CAB-CBB
18	B	827	CLA	C1A-C2A-CAA-CBA
18	B	827	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C2A-CAA-CBA-CGA
18	B	828	CLA	C4B-C3B-CAB-CBB
18	B	829	CLA	C1A-C2A-CAA-CBA
18	B	831	CLA	C1A-C2A-CAA-CBA
18	B	831	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	C2A-CAA-CBA-CGA
18	B	837	CLA	CHA-CBD-CGD-O1D
18	B	840	CLA	C3A-C2A-CAA-CBA
18	B	840	CLA	CHA-CBD-CGD-O1D
18	B	840	CLA	CHA-CBD-CGD-O2D
18	B	840	CLA	CAD-CBD-CGD-O1D
18	B	840	CLA	CAD-CBD-CGD-O2D
18	B	840	CLA	C6-C7-C8-C9
18	F	301	CLA	C3A-C2A-CAA-CBA
18	G	204	CLA	CBD-CGD-O2D-CED
18	G	204	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	C1A-C2A-CAA-CBA
18	H	201	CLA	C2B-C3B-CAB-CBB
18	H	201	CLA	C4B-C3B-CAB-CBB
18	H	201	CLA	CHA-CBD-CGD-O1D
18	H	201	CLA	CBD-CGD-O2D-CED
18	J	102	CLA	C1A-C2A-CAA-CBA
18	J	102	CLA	C3A-C2A-CAA-CBA
18	J	102	CLA	CAD-CBD-CGD-O1D
18	J	102	CLA	CAD-CBD-CGD-O2D
18	K	202	CLA	C1A-C2A-CAA-CBA
18	K	203	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	K	203	CLA	C3A-C2A-CAA-CBA
18	L	302	CLA	C1A-C2A-CAA-CBA
18	L	302	CLA	C3A-C2A-CAA-CBA
18	L	302	CLA	CHA-CBD-CGD-O1D
18	L	302	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	C1-C2-C3-C4
18	L	303	CLA	C1-C2-C3-C5
18	L	304	CLA	C1A-C2A-CAA-CBA
19	3	614	LUT	C27-C28-C29-C30
19	3	614	LUT	C27-C28-C29-C39
21	2	618	BCR	C7-C8-C9-C10
21	2	618	BCR	C11-C12-C13-C14
21	2	618	BCR	C11-C12-C13-C35
21	2	618	BCR	C17-C18-C19-C20
21	2	618	BCR	C36-C18-C19-C20
21	A	845	BCR	C23-C24-C25-C26
21	A	845	BCR	C23-C24-C25-C30
21	A	846	BCR	C36-C18-C19-C20
21	A	846	BCR	C23-C24-C25-C30
21	A	848	BCR	C21-C22-C23-C24
21	A	848	BCR	C37-C22-C23-C24
21	A	850	BCR	C11-C12-C13-C35
21	B	843	BCR	C7-C8-C9-C34
21	J	101	BCR	C22-C23-C24-C25
21	J	101	BCR	C23-C24-C25-C26
21	K	204	BCR	C23-C24-C25-C26
21	K	204	BCR	C23-C24-C25-C30
21	L	301	BCR	C1-C6-C7-C8
21	L	301	BCR	C21-C22-C23-C24
21	L	301	BCR	C37-C22-C23-C24
21	L	306	BCR	C23-C24-C25-C26
22	1	618	LHG	C4-O6-P-O5
22	1	621	LHG	O9-C7-O7-C5
22	1	621	LHG	C8-C7-O7-C5
22	1	621	LHG	O10-C23-O8-C6
22	1	621	LHG	C24-C23-O8-C6
22	1	622	LHG	C3-O3-P-O4
22	1	622	LHG	C3-O3-P-O5
22	2	617	LHG	C4-O6-P-O4
22	A	855	LHG	C3-O3-P-O4
22	A	855	LHG	C4-O6-P-O4
23	1	623	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
23	1	623	LMG	O10-C28-O8-C9
23	1	623	LMG	C29-C28-O8-C9
23	B	849	LMG	O9-C10-O7-C8
23	B	849	LMG	C11-C10-O7-C8
23	B	849	LMG	O10-C28-O8-C9
23	B	849	LMG	C29-C28-O8-C9
23	F	306	LMG	C2-C1-O1-C7
23	F	306	LMG	O6-C1-O1-C7
23	F	306	LMG	O9-C10-O7-C8
23	F	306	LMG	C11-C10-O7-C8
23	F	306	LMG	O10-C28-O8-C9
23	F	306	LMG	C29-C28-O8-C9
24	4	620	LMT	C2-C1-O1'-C1'
24	A	853	LMT	C2'-C1'-O1'-C1
24	A	853	LMT	O5'-C1'-O1'-C1
24	A	853	LMT	C2-C1-O1'-C1'
24	A	856	LMT	O5'-C1'-O1'-C1
24	G	201	LMT	C2'-C1'-O1'-C1
24	G	201	LMT	O5'-C1'-O1'-C1
27	B	848	DGD	C2B-C1B-O2G-C2G
27	B	848	DGD	O1B-C1B-O2G-C2G
17	2	614	CHL	O1D-CGD-O2D-CED
18	4	604	CLA	O1D-CGD-O2D-CED
18	F	304	CLA	O1D-CGD-O2D-CED
18	B	812	CLA	C10-C11-C12-C13
24	A	856	LMT	C3'-C4'-O1B-C1B
18	1	605	CLA	O1D-CGD-O2D-CED
18	1	611	CLA	O1D-CGD-O2D-CED
18	3	603	CLA	O1D-CGD-O2D-CED
18	3	610	CLA	O1D-CGD-O2D-CED
18	L	304	CLA	O1D-CGD-O2D-CED
17	2	605	CHL	CBD-CGD-O2D-CED
17	2	606	CHL	CBD-CGD-O2D-CED
17	4	606	CHL	CBD-CGD-O2D-CED
18	1	602	CLA	CBD-CGD-O2D-CED
18	1	605	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	CBD-CGD-O2D-CED
18	3	602	CLA	CBD-CGD-O2D-CED
18	3	605	CLA	CBD-CGD-O2D-CED
18	3	609	CLA	CBD-CGD-O2D-CED
18	4	604	CLA	CBD-CGD-O2D-CED
18	4	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	A	822	CLA	CBD-CGD-O2D-CED
18	A	823	CLA	CBD-CGD-O2D-CED
18	A	833	CLA	CBD-CGD-O2D-CED
18	B	801	CLA	CBD-CGD-O2D-CED
18	F	304	CLA	CBD-CGD-O2D-CED
18	J	102	CLA	CBD-CGD-O2D-CED
18	L	304	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	O1A-CGA-O2A-C1
17	3	616	CHL	O1A-CGA-O2A-C1
18	A	822	CLA	O1D-CGD-O2D-CED
18	J	102	CLA	O1D-CGD-O2D-CED
24	A	853	LMT	O5B-C1B-O1B-C4'
17	2	606	CHL	O1D-CGD-O2D-CED
18	3	605	CLA	O1D-CGD-O2D-CED
18	A	821	CLA	O1D-CGD-O2D-CED
18	A	825	CLA	CBA-CGA-O2A-C1
18	A	842	CLA	CBA-CGA-O2A-C1
18	F	301	CLA	CBA-CGA-O2A-C1
18	1	614	CLA	CBD-CGD-O2D-CED
18	3	617	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	CBD-CGD-O2D-CED
18	B	805	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	CBD-CGD-O2D-CED
18	B	814	CLA	CBD-CGD-O2D-CED
18	B	818	CLA	CBD-CGD-O2D-CED
18	B	831	CLA	CBD-CGD-O2D-CED
18	B	833	CLA	CBD-CGD-O2D-CED
18	4	612	CLA	O1A-CGA-O2A-C1
18	A	817	CLA	O1A-CGA-O2A-C1
18	A	819	CLA	O1A-CGA-O2A-C1
18	A	842	CLA	O1A-CGA-O2A-C1
18	B	808	CLA	O1A-CGA-O2A-C1
18	B	840	CLA	O1A-CGA-O2A-C1
18	H	201	CLA	O1A-CGA-O2A-C1
18	3	605	CLA	C2-C1-O2A-CGA
18	F	301	CLA	O1A-CGA-O2A-C1
17	1	601	CHL	C3-C5-C6-C7
18	2	604	CLA	C3-C5-C6-C7
18	A	840	CLA	C3-C5-C6-C7
18	B	805	CLA	C3-C5-C6-C7
18	B	818	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	B	839	CLA	C3-C5-C6-C7
18	F	301	CLA	C3-C5-C6-C7
18	A	819	CLA	CBA-CGA-O2A-C1
18	A	833	CLA	CBA-CGA-O2A-C1
18	B	812	CLA	CBA-CGA-O2A-C1
18	B	840	CLA	CBA-CGA-O2A-C1
18	H	201	CLA	CBA-CGA-O2A-C1
18	A	823	CLA	O1D-CGD-O2D-CED
18	A	854	CLA	C2C-C3C-CAC-CBC
18	B	817	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	C4-C3-C5-C6
18	4	609	CLA	C2-C3-C5-C6
18	A	804	CLA	C2-C3-C5-C6
18	F	301	CLA	C2-C3-C5-C6
18	L	303	CLA	CBD-CGD-O2D-CED
17	4	607	CHL	C2A-CAA-CBA-CGA
18	1	612	CLA	C2A-CAA-CBA-CGA
18	3	611	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C2A-CAA-CBA-CGA
18	A	816	CLA	C2A-CAA-CBA-CGA
18	A	817	CLA	C2A-CAA-CBA-CGA
18	A	818	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	C2A-CAA-CBA-CGA
18	A	837	CLA	C2A-CAA-CBA-CGA
18	A	839	CLA	C2A-CAA-CBA-CGA
18	B	819	CLA	C2A-CAA-CBA-CGA
18	B	823	CLA	C2A-CAA-CBA-CGA
18	L	304	CLA	C2A-CAA-CBA-CGA
18	A	812	CLA	C3-C5-C6-C7
18	A	829	CLA	C3-C5-C6-C7
18	B	833	CLA	C3-C5-C6-C7
18	3	610	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	CBA-CGA-O2A-C1
18	A	817	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	CBA-CGA-O2A-C1
18	B	808	CLA	CBA-CGA-O2A-C1
18	B	817	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C1-C2-C3-C5
18	B	820	CLA	C1-C2-C3-C5
17	4	606	CHL	O1D-CGD-O2D-CED
18	A	814	CLA	O1D-CGD-O2D-CED
18	H	201	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
18	3	617	CLA	O1A-CGA-O2A-C1
18	A	806	CLA	O1A-CGA-O2A-C1
18	A	832	CLA	O1A-CGA-O2A-C1
18	B	805	CLA	O1A-CGA-O2A-C1
18	1	614	CLA	O1D-CGD-O2D-CED
21	2	618	BCR	C9-C10-C11-C12
18	A	854	CLA	C4C-C3C-CAC-CBC
18	4	603	CLA	CBD-CGD-O2D-CED
18	B	817	CLA	CBD-CGD-O2D-CED
18	1	612	CLA	CBA-CGA-O2A-C1
18	B	805	CLA	CBA-CGA-O2A-C1
18	B	809	CLA	CBA-CGA-O2A-C1
18	B	814	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	O1A-CGA-O2A-C1
18	K	203	CLA	CBA-CGA-O2A-C1
18	3	608	CLA	CBD-CGD-O2D-CED
18	A	829	CLA	O1A-CGA-O2A-C1
18	A	833	CLA	O1A-CGA-O2A-C1
18	B	807	CLA	C3-C5-C6-C7
18	3	605	CLA	O1A-CGA-O2A-C1
18	A	804	CLA	O1A-CGA-O2A-C1
18	A	821	CLA	O1A-CGA-O2A-C1
18	B	820	CLA	C5-C6-C7-C8
18	A	824	CLA	C4-C3-C5-C6
18	B	817	CLA	C2-C3-C5-C6
18	1	614	CLA	C2A-CAA-CBA-CGA
18	3	605	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C2A-CAA-CBA-CGA
18	L	302	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	CBA-CGA-O2A-C1
18	4	612	CLA	O1D-CGD-O2D-CED
17	1	601	CHL	C1-C2-C3-C5
18	A	833	CLA	C1-C2-C3-C5
18	A	834	CLA	O1D-CGD-O2D-CED
18	B	801	CLA	O1D-CGD-O2D-CED
18	B	801	CLA	C5-C6-C7-C8
18	2	602	CLA	O1D-CGD-O2D-CED
18	3	605	CLA	CBA-CGA-O2A-C1
18	3	617	CLA	CBA-CGA-O2A-C1
18	A	806	CLA	CBA-CGA-O2A-C1
18	A	808	CLA	CBA-CGA-O2A-C1
18	A	830	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	832	CLA	CBA-CGA-O2A-C1
18	B	828	CLA	CBA-CGA-O2A-C1
18	A	817	CLA	C10-C11-C12-C13
17	1	601	CHL	C5-C6-C7-C8
18	1	608	CLA	C10-C11-C12-C13
18	A	819	CLA	C5-C6-C7-C8
18	A	833	CLA	C8-C10-C11-C12
18	B	807	CLA	C15-C16-C17-C18
18	B	831	CLA	C15-C16-C17-C18
18	B	840	CLA	C8-C10-C11-C12
24	A	856	LMT	C2'-C1'-O1'-C1
18	A	818	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	C2-C3-C5-C6
18	1	608	CLA	C14-C13-C15-C16
18	1	612	CLA	C11-C10-C8-C9
18	4	612	CLA	C6-C7-C8-C9
18	A	802	CLA	C14-C13-C15-C16
18	A	807	CLA	C14-C13-C15-C16
18	A	817	CLA	C11-C10-C8-C9
18	A	825	CLA	C11-C12-C13-C14
18	A	826	CLA	C6-C7-C8-C9
18	A	826	CLA	C14-C13-C15-C16
18	A	828	CLA	C11-C10-C8-C9
18	A	828	CLA	C11-C12-C13-C14
18	A	834	CLA	C11-C10-C8-C9
18	A	840	CLA	C11-C12-C13-C14
18	A	841	CLA	C11-C12-C13-C14
18	A	842	CLA	C11-C12-C13-C14
18	B	801	CLA	C11-C12-C13-C14
18	B	802	CLA	C6-C7-C8-C9
18	B	809	CLA	C6-C7-C8-C9
18	B	813	CLA	C14-C13-C15-C16
18	B	816	CLA	C11-C10-C8-C9
18	B	825	CLA	C11-C12-C13-C14
18	B	827	CLA	C14-C13-C15-C16
18	B	831	CLA	C14-C13-C15-C16
18	B	839	CLA	C11-C10-C8-C9
18	B	840	CLA	C14-C13-C15-C16
18	L	303	CLA	C11-C10-C8-C9
25	A	844	PQN	C19-C18-C20-C21
25	A	844	PQN	C24-C23-C25-C26
25	B	841	PQN	C19-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
18	A	833	CLA	O1D-CGD-O2D-CED
18	A	814	CLA	CBD-CGD-O2D-CED
18	A	806	CLA	C13-C15-C16-C17
18	B	815	CLA	C5-C6-C7-C8
18	A	803	CLA	C2A-CAA-CBA-CGA
18	B	838	CLA	C2A-CAA-CBA-CGA
21	2	618	BCR	C7-C8-C9-C34
21	B	843	BCR	C7-C8-C9-C10
23	1	620	LMG	C28-C29-C30-C31
17	2	607	CHL	O1A-CGA-O2A-C1
18	B	804	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	O1A-CGA-O2A-C1
18	B	837	CLA	O1A-CGA-O2A-C1
18	3	602	CLA	C10-C11-C12-C13
18	A	806	CLA	C10-C11-C12-C13
18	A	826	CLA	C15-C16-C17-C18
18	B	805	CLA	C10-C11-C12-C13
18	L	303	CLA	C10-C11-C12-C13
18	4	612	CLA	C8-C10-C11-C12
18	A	804	CLA	CBA-CGA-O2A-C1
18	A	812	CLA	CBA-CGA-O2A-C1
18	A	818	CLA	CBA-CGA-O2A-C1
18	A	829	CLA	CBA-CGA-O2A-C1
18	A	803	CLA	C10-C11-C12-C13
18	A	807	CLA	C10-C11-C12-C13
18	A	821	CLA	C15-C16-C17-C18
18	A	826	CLA	C5-C6-C7-C8
18	A	828	CLA	C5-C6-C7-C8
18	A	843	CLA	C8-C10-C11-C12
18	B	802	CLA	C8-C10-C11-C12
18	B	804	CLA	C10-C11-C12-C13
18	B	840	CLA	C5-C6-C7-C8
18	1	609	CLA	C10-C11-C12-C13
18	2	602	CLA	C10-C11-C12-C13
18	4	610	CLA	C10-C11-C12-C13
18	4	612	CLA	C5-C6-C7-C8
18	A	806	CLA	C15-C16-C17-C18
18	A	811	CLA	C15-C16-C17-C18
18	B	802	CLA	C10-C11-C12-C13
18	B	817	CLA	C5-C6-C7-C8
18	B	822	CLA	C5-C6-C7-C8
18	B	838	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	A	830	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	O1A-CGA-O2A-C1
17	2	605	CHL	O1D-CGD-O2D-CED
18	A	802	CLA	C10-C11-C12-C13
18	A	828	CLA	C15-C16-C17-C18
18	B	838	CLA	C15-C16-C17-C18
24	4	620	LMT	C5'-C4'-O1B-C1B
18	A	841	CLA	C15-C16-C17-C18
18	3	602	CLA	C5-C6-C7-C8
18	A	827	CLA	C10-C11-C12-C13
18	A	834	CLA	C5-C6-C7-C8
18	A	842	CLA	C10-C11-C12-C13
18	1	602	CLA	C11-C10-C8-C7
18	A	806	CLA	C12-C13-C15-C16
18	A	807	CLA	C11-C12-C13-C15
18	A	811	CLA	C11-C12-C13-C15
18	A	833	CLA	C12-C13-C15-C16
18	A	842	CLA	C12-C13-C15-C16
18	A	843	CLA	C12-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C15
18	B	831	CLA	C11-C12-C13-C15
25	B	841	PQN	C16-C17-C18-C20
25	B	841	PQN	C21-C22-C23-C25
18	A	826	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	O1A-CGA-O2A-C1
18	3	607	CLA	C2A-CAA-CBA-CGA
18	G	202	CLA	C2A-CAA-CBA-CGA
18	H	201	CLA	C2A-CAA-CBA-CGA
18	3	602	CLA	O1D-CGD-O2D-CED
18	1	602	CLA	C5-C6-C7-C8
18	1	612	CLA	C15-C16-C17-C18
18	A	830	CLA	C10-C11-C12-C13
18	A	842	CLA	C5-C6-C7-C8
18	A	807	CLA	O1A-CGA-O2A-C1
18	1	608	CLA	C5-C6-C7-C8
18	1	610	CLA	C5-C6-C7-C8
18	B	814	CLA	C5-C6-C7-C8
18	A	812	CLA	C5-C6-C7-C8
18	A	802	CLA	C8-C10-C11-C12
18	A	828	CLA	C10-C11-C12-C13
18	B	807	CLA	C5-C6-C7-C8
18	B	813	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	A	841	CLA	O1D-CGD-O2D-CED
18	A	808	CLA	O1A-CGA-O2A-C1
18	B	809	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	C5-C6-C7-C8
18	A	819	CLA	C13-C15-C16-C17
18	A	838	CLA	C5-C6-C7-C8
18	B	823	CLA	C13-C15-C16-C17
18	B	825	CLA	C10-C11-C12-C13
18	A	843	CLA	CBD-CGD-O2D-CED
18	B	810	CLA	C5-C6-C7-C8
18	B	822	CLA	C8-C10-C11-C12
18	B	828	CLA	C5-C6-C7-C8
18	3	617	CLA	C1-C2-C3-C5
22	1	622	LHG	C3-O3-P-O6
22	2	617	LHG	C4-O6-P-O3
22	A	852	LHG	C3-O3-P-O6
22	A	855	LHG	C3-O3-P-O6
22	A	855	LHG	C4-O6-P-O3
18	4	609	CLA	C3-C5-C6-C7
18	L	303	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C8-C10-C11-C12
18	A	825	CLA	C15-C16-C17-C18
18	A	830	CLA	C5-C6-C7-C8
18	B	839	CLA	C15-C16-C17-C18
18	4	613	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C4-C3-C5-C6
18	4	610	CLA	C5-C6-C7-C8
18	A	840	CLA	C5-C6-C7-C8
18	B	801	CLA	C10-C11-C12-C13
18	B	804	CLA	C13-C15-C16-C17
18	B	823	CLA	C5-C6-C7-C8
18	B	826	CLA	C10-C11-C12-C13
18	3	603	CLA	C2A-CAA-CBA-CGA
18	4	612	CLA	C2A-CAA-CBA-CGA
18	A	841	CLA	C2A-CAA-CBA-CGA
18	A	843	CLA	C2A-CAA-CBA-CGA
18	B	808	CLA	C2A-CAA-CBA-CGA
18	B	809	CLA	C2A-CAA-CBA-CGA
18	G	204	CLA	C2A-CAA-CBA-CGA
18	A	807	CLA	C16-C17-C18-C20
18	2	612	CLA	CBA-CGA-O2A-C1
18	B	827	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	843	CLA	C5-C6-C7-C8
18	B	817	CLA	C10-C11-C12-C13
18	B	805	CLA	C5-C6-C7-C8
18	3	602	CLA	C3-C5-C6-C7
18	L	303	CLA	C3-C5-C6-C7
18	A	824	CLA	O1D-CGD-O2D-CED
18	3	617	CLA	C6-C7-C8-C10
18	A	824	CLA	C6-C7-C8-C9
18	A	833	CLA	C16-C17-C18-C20
18	B	807	CLA	C16-C17-C18-C20
18	A	826	CLA	CBA-CGA-O2A-C1
17	4	607	CHL	C1-C2-C3-C4
18	A	808	CLA	C1-C2-C3-C5
18	A	831	CLA	C1-C2-C3-C5
18	B	824	CLA	C1-C2-C3-C5
18	B	835	CLA	C1-C2-C3-C5
18	A	834	CLA	C2C-C3C-CAC-CBC
18	A	833	CLA	C15-C16-C17-C18
18	B	813	CLA	C15-C16-C17-C18
27	B	848	DGD	C4A-C5A-C6A-C7A
18	B	833	CLA	O1D-CGD-O2D-CED
23	1	620	LMG	C2-C1-O1-C7
18	B	822	CLA	CBA-CGA-O2A-C1
17	2	601	CHL	O1A-CGA-O2A-C1
18	A	813	CLA	C10-C11-C12-C13
18	B	820	CLA	C6-C7-C8-C9
18	L	303	CLA	C11-C12-C13-C15
18	B	822	CLA	O1D-CGD-O2D-CED
18	B	807	CLA	C4-C3-C5-C6
22	A	855	LHG	C9-C10-C11-C12
18	4	612	CLA	C2-C3-C5-C6
18	4	602	CLA	C11-C10-C8-C9
18	A	801	CLA	C11-C12-C13-C14
18	A	811	CLA	C11-C10-C8-C9
18	A	817	CLA	C6-C7-C8-C9
18	A	830	CLA	C11-C12-C13-C14
18	B	802	CLA	C11-C10-C8-C9
25	B	841	PQN	C21-C22-C23-C24
23	4	619	LMG	C31-C32-C33-C34
18	1	613	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
18	A	831	CLA	C2A-CAA-CBA-CGA
18	B	821	CLA	O1A-CGA-O2A-C1
21	A	850	BCR	C11-C12-C13-C14
23	4	619	LMG	C28-C29-C30-C31
24	4	620	LMT	C3'-C4'-O1B-C1B
18	3	617	CLA	C6-C7-C8-C9
18	A	806	CLA	C16-C17-C18-C20
18	A	807	CLA	C16-C17-C18-C19
18	A	833	CLA	C16-C17-C18-C19
18	B	836	CLA	C16-C17-C18-C20
18	3	603	CLA	C5-C6-C7-C8
18	B	805	CLA	C8-C10-C11-C12
18	3	609	CLA	O1D-CGD-O2D-CED
18	4	609	CLA	C5-C6-C7-C8
23	1	623	LMG	C36-C37-C38-C39
18	4	601	CLA	CBA-CGA-O2A-C1
18	A	819	CLA	CBD-CGD-O2D-CED
27	B	848	DGD	C1B-C2B-C3B-C4B
18	A	842	CLA	C13-C15-C16-C17
18	A	840	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	O1D-CGD-O2D-CED
17	2	607	CHL	CBA-CGA-O2A-C1
18	A	801	CLA	CBA-CGA-O2A-C1
18	A	839	CLA	CBA-CGA-O2A-C1
18	K	203	CLA	O1D-CGD-O2D-CED
17	4	606	CHL	C3A-C2A-CAA-CBA
18	4	603	CLA	C3A-C2A-CAA-CBA
18	4	610	CLA	C3A-C2A-CAA-CBA
18	A	804	CLA	C3A-C2A-CAA-CBA
18	A	817	CLA	C3A-C2A-CAA-CBA
18	B	808	CLA	C3A-C2A-CAA-CBA
18	B	819	CLA	C3A-C2A-CAA-CBA
18	B	825	CLA	C3A-C2A-CAA-CBA
18	B	829	CLA	C3A-C2A-CAA-CBA
18	B	832	CLA	C3A-C2A-CAA-CBA
18	H	201	CLA	C3A-C2A-CAA-CBA
18	L	304	CLA	C3A-C2A-CAA-CBA
23	B	849	LMG	C14-C15-C16-C17
18	B	836	CLA	O1A-CGA-O2A-C1
18	B	836	CLA	C16-C17-C18-C19
22	A	852	LHG	C4-C5-C6-O8
23	1	623	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
18	1	603	CLA	CBD-CGD-O2D-CED
18	A	839	CLA	CBD-CGD-O2D-CED
18	B	802	CLA	O2A-C1-C2-C3
18	1	608	CLA	C3-C5-C6-C7
18	B	807	CLA	C13-C15-C16-C17
18	A	825	CLA	C4-C3-C5-C6
18	A	842	CLA	C4-C3-C5-C6
18	A	806	CLA	C2-C3-C5-C6
18	A	807	CLA	C2-C3-C5-C6
18	A	825	CLA	C2-C3-C5-C6
18	B	828	CLA	C2-C3-C5-C6
18	B	840	CLA	C2-C3-C5-C6
18	B	840	CLA	C1-C2-C3-C5
18	B	805	CLA	C2A-CAA-CBA-CGA
23	1	620	LMG	C22-C23-C24-C25
18	B	820	CLA	C6-C7-C8-C10
18	B	827	CLA	C16-C17-C18-C20
18	B	828	CLA	C2B-C3B-CAB-CBB
18	A	811	CLA	CBA-CGA-O2A-C1
18	B	801	CLA	O1A-CGA-O2A-C1
18	A	834	CLA	CBD-CGD-O2D-CED
23	1	623	LMG	O6-C5-C6-O5
18	B	822	CLA	C2-C1-O2A-CGA
18	B	828	CLA	O1A-CGA-O2A-C1
18	2	612	CLA	C3-C5-C6-C7
18	A	838	CLA	C3-C5-C6-C7
18	B	838	CLA	C3-C5-C6-C7
19	1	619	LUT	C1-C6-C7-C8
19	1	619	LUT	C5-C6-C7-C8
21	2	618	BCR	C1-C6-C7-C8
21	2	618	BCR	C5-C6-C7-C8
21	2	618	BCR	C23-C24-C25-C26
21	2	618	BCR	C23-C24-C25-C30
21	4	618	BCR	C23-C24-C25-C26
21	4	618	BCR	C23-C24-C25-C30
21	A	845	BCR	C1-C6-C7-C8
21	A	846	BCR	C23-C24-C25-C26
21	A	850	BCR	C5-C6-C7-C8
21	J	101	BCR	C23-C24-C25-C30
21	K	205	BCR	C23-C24-C25-C26
21	K	205	BCR	C23-C24-C25-C30
21	L	301	BCR	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	L	305	BCR	C23-C24-C25-C26
21	L	305	BCR	C23-C24-C25-C30
21	L	306	BCR	C23-C24-C25-C30
21	L	307	BCR	C1-C6-C7-C8
21	L	307	BCR	C5-C6-C7-C8
18	B	811	CLA	C2A-CAA-CBA-CGA
18	B	831	CLA	CBA-CGA-O2A-C1
18	1	602	CLA	C10-C11-C12-C13
18	2	602	CLA	C15-C16-C17-C18
18	A	804	CLA	C5-C6-C7-C8
18	A	842	CLA	C15-C16-C17-C18
18	B	809	CLA	C15-C16-C17-C18
18	B	836	CLA	C15-C16-C17-C18
18	1	602	CLA	C14-C13-C15-C16
18	A	810	CLA	O1D-CGD-O2D-CED
18	G	202	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	C2-C3-C5-C6
18	4	602	CLA	C11-C10-C8-C7
18	4	612	CLA	C6-C7-C8-C10
18	A	801	CLA	C11-C12-C13-C15
18	A	801	CLA	C12-C13-C15-C16
18	A	811	CLA	C11-C10-C8-C7
18	A	817	CLA	C6-C7-C8-C10
18	A	828	CLA	C11-C10-C8-C7
18	A	828	CLA	C11-C12-C13-C15
18	A	830	CLA	C11-C12-C13-C15
18	A	842	CLA	C2-C3-C5-C6
18	B	801	CLA	C2-C3-C5-C6
18	B	802	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C10-C8-C7
18	B	804	CLA	C11-C12-C13-C15
18	B	805	CLA	C11-C10-C8-C7
18	B	805	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C12-C13-C15
18	B	833	CLA	C2-C3-C5-C6
18	B	839	CLA	C11-C10-C8-C7
25	A	844	PQN	C17-C18-C20-C21
25	B	841	PQN	C17-C18-C20-C21
18	A	802	CLA	O1A-CGA-O2A-C1
18	A	810	CLA	O1A-CGA-O2A-C1
18	2	604	CLA	C15-C16-C17-C18
18	A	817	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	A	824	CLA	C6-C7-C8-C10
18	B	817	CLA	C11-C12-C13-C14
18	K	203	CLA	O1A-CGA-O2A-C1
18	A	807	CLA	CBA-CGA-O2A-C1
18	B	804	CLA	CBA-CGA-O2A-C1
18	B	836	CLA	CBA-CGA-O2A-C1
18	B	837	CLA	CBA-CGA-O2A-C1
17	3	616	CHL	C2A-CAA-CBA-CGA
18	A	828	CLA	C2A-CAA-CBA-CGA
18	K	203	CLA	C2A-CAA-CBA-CGA
18	A	809	CLA	CBD-CGD-O2D-CED
18	4	614	CLA	CBA-CGA-O2A-C1
18	A	821	CLA	C16-C17-C18-C20
23	1	620	LMG	O6-C1-O1-C7
18	A	843	CLA	C15-C16-C17-C18
18	B	833	CLA	C5-C6-C7-C8
18	B	816	CLA	C10-C11-C12-C13
18	B	839	CLA	C10-C11-C12-C13
18	4	614	CLA	CBD-CGD-O2D-CED
18	B	812	CLA	CBD-CGD-O2D-CED
18	4	610	CLA	C3-C5-C6-C7
23	4	621	LMG	C2-C1-O1-C7
22	1	618	LHG	O7-C5-C6-O8
23	F	306	LMG	O1-C7-C8-O7
18	1	608	CLA	C8-C10-C11-C12
18	1	612	CLA	C5-C6-C7-C8
18	B	801	CLA	C4-C3-C5-C6
18	B	805	CLA	C4-C3-C5-C6
18	B	816	CLA	C2-C3-C5-C6
18	1	602	CLA	C11-C12-C13-C14
18	1	608	CLA	C11-C10-C8-C9
18	1	612	CLA	C14-C13-C15-C16
18	A	806	CLA	C14-C13-C15-C16
18	A	811	CLA	C11-C12-C13-C14
18	A	813	CLA	C11-C10-C8-C9
18	A	819	CLA	C14-C13-C15-C16
18	A	825	CLA	C11-C10-C8-C9
18	A	833	CLA	C14-C13-C15-C16
18	B	804	CLA	C11-C12-C13-C14
18	B	812	CLA	C6-C7-C8-C9
18	B	828	CLA	C6-C7-C8-C9
18	B	831	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	841	PQN	C16-C17-C18-C19
18	1	610	CLA	CBD-CGD-O2D-CED
18	2	612	CLA	C2A-CAA-CBA-CGA
18	B	826	CLA	C2A-CAA-CBA-CGA
18	B	802	CLA	CBA-CGA-O2A-C1
17	2	614	CHL	C3A-C2A-CAA-CBA
17	4	615	CHL	C3A-C2A-CAA-CBA
18	A	832	CLA	O1D-CGD-O2D-CED
18	B	838	CLA	C8-C10-C11-C12
18	A	812	CLA	O1A-CGA-O2A-C1
18	2	613	CLA	C1A-C2A-CAA-CBA
18	4	603	CLA	C1A-C2A-CAA-CBA
18	A	804	CLA	C1A-C2A-CAA-CBA
18	A	816	CLA	C1A-C2A-CAA-CBA
18	A	818	CLA	C1A-C2A-CAA-CBA
18	A	819	CLA	C1A-C2A-CAA-CBA
18	A	824	CLA	C1A-C2A-CAA-CBA
18	A	835	CLA	C1A-C2A-CAA-CBA
18	B	802	CLA	C1A-C2A-CAA-CBA
18	B	804	CLA	C1A-C2A-CAA-CBA
18	B	808	CLA	C1A-C2A-CAA-CBA
18	B	812	CLA	C1A-C2A-CAA-CBA
18	B	817	CLA	C1A-C2A-CAA-CBA
18	B	826	CLA	C1A-C2A-CAA-CBA
18	B	832	CLA	C1A-C2A-CAA-CBA
18	B	840	CLA	C1A-C2A-CAA-CBA
18	F	301	CLA	C1A-C2A-CAA-CBA
18	G	202	CLA	C1A-C2A-CAA-CBA
18	L	303	CLA	C1A-C2A-CAA-CBA
18	A	821	CLA	C16-C17-C18-C19
18	B	827	CLA	C16-C17-C18-C19
18	L	303	CLA	C11-C12-C13-C14
18	B	838	CLA	C10-C11-C12-C13
22	1	621	LHG	C4-O6-P-O3
23	B	849	LMG	O6-C5-C6-O5
24	A	856	LMT	O5B-C5B-C6B-O6B
18	B	820	CLA	C3-C5-C6-C7
18	A	818	CLA	C10-C11-C12-C13
18	A	811	CLA	C10-C11-C12-C13
18	A	813	CLA	C8-C10-C11-C12
18	L	302	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
18	B	822	CLA	C10-C11-C12-C13
18	B	805	CLA	O1D-CGD-O2D-CED
18	1	608	CLA	C15-C16-C17-C18
18	A	813	CLA	C15-C16-C17-C18
18	4	614	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C6-C7-C8-C9
18	B	839	CLA	C16-C17-C18-C19
18	A	825	CLA	C3-C5-C6-C7
22	1	621	LHG	C4-C5-C6-O8
23	4	621	LMG	C7-C8-C9-O8
23	1	620	LMG	C8-C7-O1-C1
18	A	840	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C5-C6-C7-C8
18	3	608	CLA	O1D-CGD-O2D-CED
18	B	816	CLA	C11-C12-C13-C14
18	4	602	CLA	CBD-CGD-O2D-CED
24	A	856	LMT	O5'-C5'-C6'-O6'
18	A	826	CLA	C10-C11-C12-C13
18	A	834	CLA	C4-C3-C5-C6
18	B	815	CLA	C4-C3-C5-C6
18	G	202	CLA	CBD-CGD-O2D-CED
18	2	604	CLA	C2A-CAA-CBA-CGA
18	B	813	CLA	C2A-CAA-CBA-CGA
18	4	614	CLA	C1-C2-C3-C5
18	3	607	CLA	O1D-CGD-O2D-CED
18	B	825	CLA	O1D-CGD-O2D-CED
18	A	834	CLA	C4C-C3C-CAC-CBC
18	1	602	CLA	O1D-CGD-O2D-CED
18	A	802	CLA	C15-C16-C17-C18
23	B	849	LMG	C21-C22-C23-C24
18	1	610	CLA	CBA-CGA-O2A-C1
18	B	821	CLA	CBA-CGA-O2A-C1
18	B	833	CLA	CBA-CGA-O2A-C1
18	2	612	CLA	O1A-CGA-O2A-C1
18	B	814	CLA	C6-C7-C8-C10
18	B	839	CLA	C16-C17-C18-C20
18	B	831	CLA	C10-C11-C12-C13
18	4	610	CLA	CAA-CBA-CGA-O2A
23	B	849	LMG	O1-C7-C8-O7
18	A	813	CLA	C1-C2-C3-C5
18	B	827	CLA	C10-C11-C12-C13
18	3	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
18	A	813	CLA	C4-C3-C5-C6
18	1	602	CLA	C11-C12-C13-C15
18	1	608	CLA	C11-C12-C13-C15
18	1	612	CLA	C12-C13-C15-C16
18	4	610	CLA	C6-C7-C8-C10
18	A	803	CLA	C6-C7-C8-C10
18	A	813	CLA	C11-C10-C8-C7
18	A	813	CLA	C12-C13-C15-C16
18	A	819	CLA	C12-C13-C15-C16
18	A	825	CLA	C11-C10-C8-C7
18	A	842	CLA	C11-C12-C13-C15
18	A	843	CLA	C11-C12-C13-C15
18	B	801	CLA	C11-C12-C13-C15
18	B	805	CLA	C2-C3-C5-C6
18	B	805	CLA	C11-C12-C13-C15
18	B	807	CLA	C11-C12-C13-C15
18	B	812	CLA	C6-C7-C8-C10
18	B	823	CLA	C11-C10-C8-C7
18	B	823	CLA	C11-C12-C13-C15
18	B	823	CLA	C12-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C7
18	B	826	CLA	C11-C10-C8-C7
18	B	828	CLA	C6-C7-C8-C10
18	B	839	CLA	C11-C12-C13-C15
18	B	839	CLA	C12-C13-C15-C16
18	B	840	CLA	C11-C10-C8-C7
18	B	840	CLA	C12-C13-C15-C16
18	A	801	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	C3-C5-C6-C7
18	3	602	CLA	C6-C7-C8-C9
18	4	610	CLA	C6-C7-C8-C9
18	A	802	CLA	C11-C10-C8-C9
18	A	807	CLA	C11-C12-C13-C14
18	A	819	CLA	C11-C12-C13-C14
18	A	840	CLA	C11-C10-C8-C9
18	A	842	CLA	C11-C10-C8-C9
18	A	842	CLA	C14-C13-C15-C16
18	A	843	CLA	C11-C12-C13-C14
18	B	801	CLA	C11-C10-C8-C9
18	B	805	CLA	C14-C13-C15-C16
18	B	809	CLA	C11-C12-C13-C14
18	B	809	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
18	B	813	CLA	C11-C10-C8-C9
18	B	823	CLA	C6-C7-C8-C9
18	B	826	CLA	C11-C10-C8-C9
18	B	840	CLA	C11-C12-C13-C14
18	F	301	CLA	C6-C7-C8-C9
18	A	813	CLA	CBA-CGA-O2A-C1
18	B	838	CLA	CBA-CGA-O2A-C1
18	2	610	CLA	O1D-CGD-O2D-CED
18	B	827	CLA	C8-C10-C11-C12
18	4	601	CLA	O1A-CGA-O2A-C1
18	B	813	CLA	CBA-CGA-O2A-C1
18	A	828	CLA	C8-C10-C11-C12
18	B	809	CLA	C5-C6-C7-C8
18	B	830	CLA	C2A-CAA-CBA-CGA
18	B	807	CLA	C16-C17-C18-C19
18	B	813	CLA	C8-C10-C11-C12
18	A	817	CLA	C1-C2-C3-C5
18	B	840	CLA	C4-C3-C5-C6
18	F	301	CLA	C4-C3-C5-C6
18	A	834	CLA	C2-C3-C5-C6
18	B	807	CLA	C2-C3-C5-C6
18	B	826	CLA	C2-C3-C5-C6
18	B	817	CLA	C8-C10-C11-C12
18	1	603	CLA	CBA-CGA-O2A-C1
18	B	801	CLA	CBA-CGA-O2A-C1
18	3	617	CLA	O1D-CGD-O2D-CED
18	A	806	CLA	C3A-C2A-CAA-CBA
18	A	818	CLA	C3A-C2A-CAA-CBA
18	A	831	CLA	C3A-C2A-CAA-CBA
18	A	837	CLA	C3A-C2A-CAA-CBA
18	B	835	CLA	C3A-C2A-CAA-CBA
18	B	839	CLA	C3A-C2A-CAA-CBA
18	B	821	CLA	C3-C5-C6-C7
18	B	805	CLA	C16-C17-C18-C19
18	B	835	CLA	CBA-CGA-O2A-C1
22	1	618	LHG	C4-C5-C6-O8
23	B	849	LMG	O1-C7-C8-C9
23	F	306	LMG	O1-C7-C8-C9
18	A	812	CLA	O2A-C1-C2-C3
18	A	831	CLA	O2A-C1-C2-C3
18	B	831	CLA	O2A-C1-C2-C3
18	A	842	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
18	A	819	CLA	C2-C3-C5-C6
18	4	613	CLA	C2A-CAA-CBA-CGA
18	A	813	CLA	C2A-CAA-CBA-CGA
18	A	821	CLA	C2A-CAA-CBA-CGA
18	A	825	CLA	C2A-CAA-CBA-CGA
18	A	803	CLA	CBA-CGA-O2A-C1
17	1	601	CHL	C6-C7-C8-C9
18	1	609	CLA	C5-C6-C7-C8
18	1	602	CLA	O1A-CGA-O2A-C1
18	1	610	CLA	O1A-CGA-O2A-C1
18	A	811	CLA	O1A-CGA-O2A-C1
23	1	623	LMG	C2-C1-O1-C7
27	B	848	DGD	O2G-C2G-C3G-O3G
18	B	805	CLA	C16-C17-C18-C20
18	B	817	CLA	C11-C12-C13-C15
18	B	824	CLA	C2-C1-O2A-CGA
18	A	818	CLA	CAA-CBA-CGA-O2A
18	2	604	CLA	C11-C10-C8-C9
18	A	803	CLA	C6-C7-C8-C9
18	A	806	CLA	C11-C10-C8-C9
18	B	817	CLA	C11-C10-C8-C9
18	B	822	CLA	C6-C7-C8-C9
18	B	823	CLA	C14-C13-C15-C16
18	B	825	CLA	C14-C13-C15-C16
18	B	838	CLA	C14-C13-C15-C16
18	B	839	CLA	C11-C12-C13-C14
18	B	840	CLA	C11-C10-C8-C9
18	A	819	CLA	C10-C11-C12-C13
17	2	601	CHL	C1A-C2A-CAA-CBA
18	3	603	CLA	C6-C7-C8-C9
18	B	812	CLA	C16-C17-C18-C19
19	2	615	LUT	C1-C6-C7-C8
21	A	845	BCR	C5-C6-C7-C8
21	A	850	BCR	C1-C6-C7-C8
21	J	103	BCR	C23-C24-C25-C26
21	J	103	BCR	C23-C24-C25-C30
21	K	205	BCR	C1-C6-C7-C8
21	K	205	BCR	C5-C6-C7-C8
18	A	830	CLA	C13-C15-C16-C17
18	2	613	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	O1A-CGA-O2A-C1
18	A	813	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
18	A	817	CLA	C11-C12-C13-C15
18	B	828	CLA	C11-C10-C8-C9
18	B	809	CLA	C10-C11-C12-C13
18	B	814	CLA	O1D-CGD-O2D-CED
18	A	830	CLA	C15-C16-C17-C18
18	B	804	CLA	C15-C16-C17-C18
22	1	618	LHG	O6-C4-C5-C6
18	1	609	CLA	C11-C10-C8-C7
18	2	604	CLA	C11-C10-C8-C7
18	3	602	CLA	C6-C7-C8-C10
18	A	806	CLA	C11-C10-C8-C7
18	A	819	CLA	C11-C12-C13-C15
18	A	825	CLA	C11-C12-C13-C15
18	A	826	CLA	C6-C7-C8-C10
18	A	827	CLA	C12-C13-C15-C16
18	A	829	CLA	C11-C12-C13-C15
18	A	840	CLA	C11-C10-C8-C7
18	A	842	CLA	C11-C10-C8-C7
18	B	801	CLA	C11-C10-C8-C7
18	B	809	CLA	C12-C13-C15-C16
18	B	813	CLA	C11-C10-C8-C7
18	B	816	CLA	C6-C7-C8-C10
18	B	816	CLA	C11-C10-C8-C7
18	B	817	CLA	C11-C10-C8-C7
18	B	823	CLA	C6-C7-C8-C10
18	B	827	CLA	C12-C13-C15-C16
18	B	838	CLA	C12-C13-C15-C16
18	B	840	CLA	C6-C7-C8-C10
18	B	840	CLA	C11-C12-C13-C15
18	F	301	CLA	C6-C7-C8-C10
17	2	607	CHL	C1C-C2C-CMC-OMC
21	2	618	BCR	C19-C20-C21-C22
18	3	603	CLA	C6-C7-C8-C10
18	A	829	CLA	C15-C16-C17-C18
18	4	608	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C16-C17-C18-C20
23	1	620	LMG	C33-C34-C35-C36
17	3	616	CHL	CBD-CGD-O2D-CED
18	1	613	CLA	CAD-CBD-CGD-O2D
18	2	602	CLA	CAD-CBD-CGD-O2D
18	2	613	CLA	CAD-CBD-CGD-O2D
18	3	609	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	3	617	CLA	CAD-CBD-CGD-O2D
18	4	603	CLA	CAD-CBD-CGD-O2D
18	4	604	CLA	CAD-CBD-CGD-O2D
18	A	808	CLA	CAD-CBD-CGD-O2D
18	A	812	CLA	CAD-CBD-CGD-O2D
18	A	823	CLA	CAD-CBD-CGD-O2D
18	A	826	CLA	CAD-CBD-CGD-O2D
18	A	830	CLA	CAD-CBD-CGD-O2D
18	B	809	CLA	CAD-CBD-CGD-O2D
18	B	819	CLA	CAD-CBD-CGD-O2D
18	B	824	CLA	CAD-CBD-CGD-O2D
18	F	303	CLA	CAD-CBD-CGD-O2D
18	G	202	CLA	CAD-CBD-CGD-O2D
22	A	852	LHG	C32-C33-C34-C35
18	A	802	CLA	C13-C15-C16-C17
21	A	847	BCR	C6-C7-C8-C9
18	A	828	CLA	CBA-CGA-O2A-C1
22	1	621	LHG	C2-C3-O3-P
18	A	801	CLA	O1A-CGA-O2A-C1
22	1	618	LHG	O6-C4-C5-O7
18	2	604	CLA	C8-C10-C11-C12
18	A	824	CLA	C5-C6-C7-C8
18	4	602	CLA	C11-C12-C13-C15
18	A	829	CLA	C16-C17-C18-C20
18	B	831	CLA	O1D-CGD-O2D-CED
18	1	604	CLA	CHA-CBD-CGD-O1D
18	2	612	CLA	CHA-CBD-CGD-O2D
18	3	602	CLA	CHA-CBD-CGD-O1D
18	3	610	CLA	CHA-CBD-CGD-O1D
18	4	603	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O1D
18	A	804	CLA	CHA-CBD-CGD-O2D
18	A	805	CLA	CHA-CBD-CGD-O1D
18	A	805	CLA	CHA-CBD-CGD-O2D
18	A	815	CLA	CHA-CBD-CGD-O1D
18	A	819	CLA	CHA-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O1D
18	A	827	CLA	CHA-CBD-CGD-O2D
18	A	831	CLA	CHA-CBD-CGD-O1D
18	A	831	CLA	CHA-CBD-CGD-O2D
18	A	836	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	B	804	CLA	CHA-CBD-CGD-O1D
18	B	804	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O1D
18	B	820	CLA	CHA-CBD-CGD-O2D
18	B	822	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O1D
18	B	832	CLA	CHA-CBD-CGD-O2D
18	B	837	CLA	CHA-CBD-CGD-O2D
18	H	201	CLA	CHA-CBD-CGD-O2D
18	B	825	CLA	O1A-CGA-O2A-C1
18	B	827	CLA	O1A-CGA-O2A-C1
23	B	849	LMG	C2-C1-O1-C7
23	B	849	LMG	C16-C17-C18-C19
23	4	621	LMG	O1-C7-C8-O7
23	4	621	LMG	O7-C8-C9-O8
18	A	825	CLA	O1D-CGD-O2D-CED
18	L	303	CLA	O1A-CGA-O2A-C1
18	B	802	CLA	O1D-CGD-O2D-CED
22	1	618	LHG	C23-C24-C25-C26
25	A	844	PQN	C16-C17-C18-C19
18	B	810	CLA	O1D-CGD-O2D-CED
18	B	814	CLA	C2A-CAA-CBA-CGA
18	A	815	CLA	CBD-CGD-O2D-CED
21	A	847	BCR	C7-C8-C9-C34
21	A	846	BCR	C17-C18-C19-C20
21	L	305	BCR	C21-C22-C23-C24
18	2	604	CLA	C1A-C2A-CAA-CBA
18	A	837	CLA	C1A-C2A-CAA-CBA
18	B	835	CLA	C1A-C2A-CAA-CBA
18	B	839	CLA	C1A-C2A-CAA-CBA
18	2	602	CLA	C16-C17-C18-C20
18	A	827	CLA	C1-C2-C3-C5
22	1	618	LHG	C4-O6-P-O3
22	A	852	LHG	C4-O6-P-O3
22	1	618	LHG	C5-C4-O6-P
18	A	806	CLA	C4B-C3B-CAB-CBB
18	B	803	CLA	C4B-C3B-CAB-CBB
18	L	303	CLA	C4B-C3B-CAB-CBB
22	A	852	LHG	C3-O3-P-O5
22	A	855	LHG	C4-O6-P-O5
18	3	602	CLA	C11-C12-C13-C15
18	A	804	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
18	A	809	CLA	C6-C7-C8-C10
23	B	849	LMG	O6-C1-O1-C7
18	A	831	CLA	CBD-CGD-O2D-CED
17	3	616	CHL	CAD-CBD-CGD-O1D
18	4	601	CLA	CAD-CBD-CGD-O1D
18	4	613	CLA	CAD-CBD-CGD-O1D
18	A	813	CLA	CAD-CBD-CGD-O1D
18	A	824	CLA	CAD-CBD-CGD-O1D
18	A	827	CLA	CAD-CBD-CGD-O1D
18	B	804	CLA	CAD-CBD-CGD-O1D
18	B	812	CLA	CAD-CBD-CGD-O1D
18	B	828	CLA	CAD-CBD-CGD-O1D
18	H	201	CLA	C2-C3-C5-C6
18	B	805	CLA	C15-C16-C17-C18
18	A	819	CLA	C16-C17-C18-C19
18	B	826	CLA	C11-C12-C13-C14
17	1	601	CHL	CAD-CBD-CGD-O2D
18	1	612	CLA	C6-C7-C8-C10
18	1	612	CLA	C11-C10-C8-C7
18	A	803	CLA	C11-C12-C13-C15
18	A	819	CLA	C6-C7-C8-C10
18	A	826	CLA	C11-C12-C13-C15
18	A	834	CLA	C11-C10-C8-C7
18	A	840	CLA	C6-C7-C8-C10
18	B	802	CLA	C12-C13-C15-C16
18	B	812	CLA	C11-C12-C13-C15
18	B	813	CLA	C11-C12-C13-C15
18	B	813	CLA	C12-C13-C15-C16
18	B	818	CLA	C3A-C2A-CAA-CBA
18	B	827	CLA	C6-C7-C8-C10
18	B	836	CLA	C12-C13-C15-C16
25	A	844	PQN	C22-C23-C25-C26
18	B	801	CLA	CAA-CBA-CGA-O2A
23	4	621	LMG	O1-C7-C8-C9
22	1	621	LHG	O7-C5-C6-O8
22	A	852	LHG	O7-C5-C6-O8
23	1	623	LMG	O7-C8-C9-O8
18	B	816	CLA	O2A-C1-C2-C3
18	A	810	CLA	CBA-CGA-O2A-C1
18	B	815	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C6-C7-C8-C9
18	A	826	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
18	A	828	CLA	C14-C13-C15-C16
18	A	829	CLA	C11-C10-C8-C9
18	A	843	CLA	C11-C10-C8-C9
18	A	843	CLA	C14-C13-C15-C16
18	B	801	CLA	C6-C7-C8-C9
18	B	816	CLA	C6-C7-C8-C9
18	2	604	CLA	O1D-CGD-O2D-CED
18	A	803	CLA	O1D-CGD-O2D-CED
18	A	809	CLA	C6-C7-C8-C9
18	3	602	CLA	C2A-CAA-CBA-CGA
21	2	618	BCR	C10-C11-C12-C13
21	A	846	BCR	C18-C19-C20-C21
21	A	850	BCR	C10-C11-C12-C13
18	A	833	CLA	C3-C5-C6-C7
18	L	303	CLA	C2B-C3B-CAB-CBB
18	4	601	CLA	CAA-CBA-CGA-O2A
18	B	833	CLA	CAA-CBA-CGA-O2A
18	2	609	CLA	C2-C3-C5-C6
18	B	836	CLA	C5-C6-C7-C8
18	B	840	CLA	C16-C17-C18-C19
18	3	617	CLA	C5-C6-C7-C8
18	A	810	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	C2A-CAA-CBA-CGA
18	B	815	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C1-C2-C3-C5
18	B	813	CLA	C1-C2-C3-C5
18	A	804	CLA	C2-C1-O2A-CGA
18	A	806	CLA	C2-C1-O2A-CGA
18	A	812	CLA	C2-C1-O2A-CGA
18	A	804	CLA	C6-C7-C8-C9
23	1	620	LMG	C17-C18-C19-C20
22	A	852	LHG	C25-C26-C27-C28
18	B	813	CLA	C4-C3-C5-C6
21	1	617	BCR	C23-C24-C25-C30
18	4	610	CLA	C8-C10-C11-C12
17	1	606	CHL	C2C-C3C-CAC-CBC
18	A	837	CLA	O1D-CGD-O2D-CED
18	A	812	CLA	CBD-CGD-O2D-CED
18	1	608	CLA	C1-C2-C3-C5
22	2	617	LHG	C3-O3-P-O6
18	B	807	CLA	O1D-CGD-O2D-CED
17	2	606	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
18	A	807	CLA	C12-C13-C15-C16
18	B	801	CLA	C6-C7-C8-C10
18	B	831	CLA	C3-C5-C6-C7
18	1	602	CLA	C11-C10-C8-C9
18	A	813	CLA	C14-C13-C15-C16
18	A	819	CLA	C6-C7-C8-C9
18	A	840	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C12-C13-C14
18	B	812	CLA	C11-C12-C13-C14
18	B	813	CLA	C11-C12-C13-C14
18	3	602	CLA	C11-C12-C13-C14
18	A	801	CLA	C15-C16-C17-C18
18	A	829	CLA	CBD-CGD-O2D-CED
18	B	801	CLA	C8-C10-C11-C12
18	B	827	CLA	C13-C15-C16-C17
18	1	602	CLA	C12-C13-C15-C16
18	B	828	CLA	C11-C10-C8-C7
23	1	623	LMG	C33-C34-C35-C36
18	A	807	CLA	C4-C3-C5-C6
18	B	826	CLA	C11-C12-C13-C15
18	B	819	CLA	CBA-CGA-O2A-C1
17	2	601	CHL	CBD-CGD-O2D-CED
23	4	621	LMG	C24-C25-C26-C27
18	A	827	CLA	O1A-CGA-O2A-C1
18	A	829	CLA	C5-C6-C7-C8
18	B	808	CLA	C5-C6-C7-C8
18	B	808	CLA	C6-C7-C8-C9
18	1	608	CLA	C4-C3-C5-C6
18	B	826	CLA	C4-C3-C5-C6
18	B	804	CLA	C5-C6-C7-C8
18	B	827	CLA	C15-C16-C17-C18
17	1	601	CHL	C2-C1-O2A-CGA
18	4	614	CLA	C2-C1-O2A-CGA
18	B	805	CLA	C2-C1-O2A-CGA
18	A	834	CLA	C8-C10-C11-C12
18	B	807	CLA	C2A-CAA-CBA-CGA
18	A	834	CLA	CBA-CGA-O2A-C1
22	2	617	LHG	C2-C3-O3-P
22	2	617	LHG	C5-C4-O6-P
18	3	604	CLA	C3A-C2A-CAA-CBA
18	A	825	CLA	C3A-C2A-CAA-CBA
18	A	839	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
18	B	809	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C3A-C2A-CAA-CBA
18	B	833	CLA	C3A-C2A-CAA-CBA
18	B	837	CLA	C3A-C2A-CAA-CBA
18	K	202	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C11-C12-C13-C14
18	1	604	CLA	O2A-C1-C2-C3
18	1	612	CLA	CBD-CGD-O2D-CED
18	A	809	CLA	C4-C3-C5-C6
18	A	801	CLA	C14-C13-C15-C16
18	A	827	CLA	C6-C7-C8-C9
18	A	841	CLA	C6-C7-C8-C9
18	A	843	CLA	C6-C7-C8-C9
18	B	802	CLA	C11-C12-C13-C14
18	B	825	CLA	C6-C7-C8-C9
18	B	809	CLA	C16-C17-C18-C19
18	2	603	CLA	CAA-CBA-CGA-O1A
18	A	816	CLA	CAA-CBA-CGA-O1A
21	A	849	BCR	C11-C10-C9-C34
21	A	849	BCR	C16-C17-C18-C36
21	A	850	BCR	C16-C17-C18-C36
21	B	844	BCR	C11-C10-C9-C34
21	B	844	BCR	C20-C21-C22-C37
21	F	305	BCR	C35-C13-C14-C15
21	L	307	BCR	C11-C10-C9-C34
18	2	608	CLA	CAA-CBA-CGA-O2A
18	A	824	CLA	C2A-CAA-CBA-CGA
18	B	812	CLA	C5-C6-C7-C8
18	B	808	CLA	C6-C7-C8-C10
25	A	844	PQN	C26-C27-C28-C30
18	B	820	CLA	O2A-C1-C2-C3
18	L	304	CLA	CAA-CBA-CGA-O1A
18	B	833	CLA	C4-C3-C5-C6
18	1	614	CLA	C1A-C2A-CAA-CBA
18	3	604	CLA	C1A-C2A-CAA-CBA
18	A	806	CLA	C1A-C2A-CAA-CBA
18	A	825	CLA	C1A-C2A-CAA-CBA
18	B	816	CLA	C1A-C2A-CAA-CBA
18	B	818	CLA	C1A-C2A-CAA-CBA
18	B	837	CLA	C1A-C2A-CAA-CBA
18	A	840	CLA	CBA-CGA-O2A-C1
18	1	612	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
18	2	604	CLA	C11-C12-C13-C15
18	4	612	CLA	C11-C10-C8-C7
18	A	840	CLA	C11-C12-C13-C15
18	A	841	CLA	C12-C13-C15-C16
18	A	843	CLA	C6-C7-C8-C10
18	B	822	CLA	C11-C10-C8-C7
18	B	816	CLA	C5-C6-C7-C8
18	A	835	CLA	CAA-CBA-CGA-O1A
18	1	614	CLA	CAA-CBA-CGA-O2A
18	A	842	CLA	C2A-CAA-CBA-CGA
18	B	806	CLA	C2A-CAA-CBA-CGA
18	G	204	CLA	CAA-CBA-CGA-O1A
18	2	603	CLA	CAA-CBA-CGA-O2A
18	A	806	CLA	C2B-C3B-CAB-CBB
18	B	803	CLA	C2B-C3B-CAB-CBB
18	B	829	CLA	C2B-C3B-CAB-CBB
18	B	838	CLA	C5-C6-C7-C8
18	A	827	CLA	O1D-CGD-O2D-CED
21	A	849	BCR	C11-C10-C9-C8
21	A	849	BCR	C16-C17-C18-C19
21	A	850	BCR	C16-C17-C18-C19
21	B	844	BCR	C11-C10-C9-C8
21	B	844	BCR	C20-C21-C22-C23
21	F	305	BCR	C12-C13-C14-C15
21	L	307	BCR	C11-C10-C9-C8
18	A	801	CLA	C8-C10-C11-C12
22	1	621	LHG	C11-C12-C13-C14
18	1	608	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	C3-C5-C6-C7
18	B	823	CLA	O1A-CGA-O2A-C1
25	B	841	PQN	C13-C15-C16-C17
18	1	609	CLA	C4-C3-C5-C6
18	2	612	CLA	C4-C3-C5-C6
18	B	820	CLA	C4-C3-C5-C6
18	A	825	CLA	C2-C1-O2A-CGA
18	A	837	CLA	C2-C1-O2A-CGA
18	B	809	CLA	C2-C1-O2A-CGA
18	B	815	CLA	C2-C3-C5-C6
18	1	611	CLA	CAA-CBA-CGA-O2A
18	2	611	CLA	CAA-CBA-CGA-O2A
18	B	836	CLA	C11-C12-C13-C14
18	2	608	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
17	2	607	CHL	C1A-C2A-CAA-CBA
18	B	839	CLA	C2A-CAA-CBA-CGA
23	4	621	LMG	C20-C21-C22-C23
18	4	602	CLA	O1A-CGA-O2A-C1
19	4	616	LUT	C1-C6-C7-C8
21	1	617	BCR	C23-C24-C25-C26
21	B	843	BCR	C1-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C30
21	J	101	BCR	C1-C6-C7-C8
18	B	818	CLA	C4-C3-C5-C6
18	3	607	CLA	CAA-CBA-CGA-O2A
18	B	816	CLA	C8-C10-C11-C12
18	A	835	CLA	CAA-CBA-CGA-O2A
18	L	304	CLA	CAA-CBA-CGA-O2A
18	2	612	CLA	C6-C7-C8-C9
22	A	852	LHG	C10-C11-C12-C13
17	4	606	CHL	CAA-CBA-CGA-O2A
18	3	604	CLA	C2A-CAA-CBA-CGA
18	B	833	CLA	C2A-CAA-CBA-CGA
18	F	301	CLA	C5-C6-C7-C8
18	3	607	CLA	CAA-CBA-CGA-O1A
18	A	816	CLA	CAA-CBA-CGA-O2A
18	B	829	CLA	C4B-C3B-CAB-CBB
18	B	801	CLA	C16-C17-C18-C19
18	1	608	CLA	C11-C10-C8-C7
22	A	852	LHG	C14-C15-C16-C17
18	A	802	CLA	C1-C2-C3-C4
18	A	818	CLA	C1-C2-C3-C4
18	A	828	CLA	C1-C2-C3-C4
18	A	840	CLA	C16-C17-C18-C19
18	G	204	CLA	CAA-CBA-CGA-O2A
23	F	306	LMG	O7-C8-C9-O8
18	1	609	CLA	O1A-CGA-O2A-C1
18	A	802	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	CAA-CBA-CGA-O2A
18	A	839	CLA	O1A-CGA-O2A-C1
18	B	822	CLA	CAA-CBA-CGA-O2A
23	1	620	LMG	C11-C12-C13-C14
18	1	603	CLA	C4-C3-C5-C6
18	2	604	CLA	C4-C3-C5-C6
18	A	827	CLA	C4-C3-C5-C6
23	B	849	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
18	4	612	CLA	C11-C10-C8-C9
18	A	803	CLA	C11-C12-C13-C14
18	A	821	CLA	C6-C7-C8-C9
18	A	830	CLA	C6-C7-C8-C9
18	B	827	CLA	C6-C7-C8-C9
18	B	836	CLA	C14-C13-C15-C16
18	B	839	CLA	C14-C13-C15-C16
18	B	817	CLA	C3-C5-C6-C7
18	1	614	CLA	C3A-C2A-CAA-CBA
18	A	811	CLA	C3A-C2A-CAA-CBA
18	A	841	CLA	C3A-C2A-CAA-CBA
18	B	816	CLA	C3A-C2A-CAA-CBA
18	B	830	CLA	C3A-C2A-CAA-CBA
18	B	831	CLA	CAA-CBA-CGA-O2A
22	1	622	LHG	O7-C7-C8-C9
18	2	611	CLA	CAA-CBA-CGA-O1A
17	2	614	CHL	CAD-CBD-CGD-O2D
18	1	604	CLA	CAD-CBD-CGD-O2D
18	2	604	CLA	CAD-CBD-CGD-O2D
18	4	602	CLA	CAD-CBD-CGD-O2D
18	A	805	CLA	CAD-CBD-CGD-O2D
18	A	807	CLA	CAD-CBD-CGD-O2D
18	A	811	CLA	CAD-CBD-CGD-O2D
18	A	814	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	CAD-CBD-CGD-O2D
18	A	820	CLA	CAD-CBD-CGD-O2D
18	A	825	CLA	CAD-CBD-CGD-O2D
18	A	834	CLA	CAD-CBD-CGD-O2D
18	A	837	CLA	CAD-CBD-CGD-O2D
18	B	810	CLA	CAD-CBD-CGD-O2D
18	B	811	CLA	CAD-CBD-CGD-O2D
18	B	812	CLA	CAD-CBD-CGD-O2D
18	B	814	CLA	CAD-CBD-CGD-O2D
18	B	829	CLA	CAD-CBD-CGD-O2D
18	B	831	CLA	CAD-CBD-CGD-O2D
18	B	834	CLA	CAD-CBD-CGD-O2D
18	B	835	CLA	CAD-CBD-CGD-O2D
18	F	301	CLA	CAD-CBD-CGD-O2D
18	K	202	CLA	CAD-CBD-CGD-O2D
18	K	203	CLA	CAD-CBD-CGD-O2D
18	L	304	CLA	CAD-CBD-CGD-O2D
18	2	603	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
23	F	306	LMG	C32-C33-C34-C35
18	A	807	CLA	C2-C1-O2A-CGA
18	A	808	CLA	C1-C2-C3-C4
18	B	832	CLA	CAA-CBA-CGA-O2A
18	B	839	CLA	C5-C6-C7-C8
18	A	843	CLA	C4-C3-C5-C6
21	2	618	BCR	C21-C22-C23-C24
27	B	848	DGD	C1G-C2G-C3G-O3G
18	K	202	CLA	CAA-CBA-CGA-O1A
18	K	202	CLA	CAA-CBA-CGA-O2A
18	A	825	CLA	CAA-CBA-CGA-O2A
18	B	840	CLA	CAA-CBA-CGA-O2A
18	2	604	CLA	O2A-C1-C2-C3
18	4	614	CLA	O2A-C1-C2-C3
18	A	808	CLA	O2A-C1-C2-C3
18	A	818	CLA	O2A-C1-C2-C3
18	A	828	CLA	O2A-C1-C2-C3
18	A	854	CLA	O2A-C1-C2-C3
18	B	821	CLA	O2A-C1-C2-C3
18	2	602	CLA	C2A-CAA-CBA-CGA
18	A	842	CLA	C8-C10-C11-C12
18	1	603	CLA	CHA-CBD-CGD-O2D
18	1	613	CLA	CHA-CBD-CGD-O1D
18	2	604	CLA	CHA-CBD-CGD-O2D
18	3	604	CLA	CHA-CBD-CGD-O2D
18	4	601	CLA	CHA-CBD-CGD-O2D
18	4	602	CLA	CHA-CBD-CGD-O2D
18	4	604	CLA	CHA-CBD-CGD-O1D
18	4	614	CLA	CHA-CBD-CGD-O2D
18	A	813	CLA	CHA-CBD-CGD-O2D
18	A	822	CLA	CHA-CBD-CGD-O1D
18	A	824	CLA	CHA-CBD-CGD-O1D
18	A	829	CLA	CHA-CBD-CGD-O2D
18	A	834	CLA	CHA-CBD-CGD-O2D
18	A	838	CLA	CHA-CBD-CGD-O1D
18	B	801	CLA	CHA-CBD-CGD-O2D
18	B	807	CLA	CHA-CBD-CGD-O2D
18	B	827	CLA	CHA-CBD-CGD-O1D
18	B	827	CLA	CHA-CBD-CGD-O2D
18	L	303	CLA	CHA-CBD-CGD-O2D
18	L	304	CLA	CHA-CBD-CGD-O1D
18	G	202	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	1	618	LHG	O7-C7-C8-C9
27	B	848	DGD	CBB-CCB-CDB-CEB
17	1	601	CHL	C6-C7-C8-C10
18	A	829	CLA	CAA-CBA-CGA-O2A
23	1	620	LMG	O8-C28-C29-C30
23	1	620	LMG	C36-C37-C38-C39
23	4	619	LMG	O7-C8-C9-O8
18	A	840	CLA	C15-C16-C17-C18
18	B	826	CLA	O1A-CGA-O2A-C1
17	3	616	CHL	CAA-CBA-CGA-O2A
18	A	804	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	CAA-CBA-CGA-O2A
18	B	817	CLA	C2A-CAA-CBA-CGA
18	A	829	CLA	C16-C17-C18-C19
18	1	611	CLA	CAA-CBA-CGA-O1A
18	B	831	CLA	C12-C13-C15-C16
18	1	608	CLA	C6-C7-C8-C9
18	B	805	CLA	C11-C10-C8-C9
18	B	822	CLA	C11-C10-C8-C9
18	1	603	CLA	CAA-CBA-CGA-O1A
18	1	613	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	CAA-CBA-CGA-O2A
18	1	608	CLA	C16-C17-C18-C20
18	A	838	CLA	C6-C7-C8-C9
18	4	604	CLA	C2A-CAA-CBA-CGA
18	2	602	CLA	C4-C3-C5-C6
18	B	822	CLA	C4-C3-C5-C6
18	A	825	CLA	CAA-CBA-CGA-O1A
18	H	201	CLA	CAA-CBA-CGA-O1A
17	1	601	CHL	CHA-CBD-CGD-O1D
17	1	601	CHL	CHA-CBD-CGD-O2D
17	1	606	CHL	CHA-CBD-CGD-O1D
18	3	606	CLA	CHA-CBD-CGD-O2D
18	3	610	CLA	C1A-C2A-CAA-CBA
18	3	611	CLA	CHA-CBD-CGD-O2D
18	A	811	CLA	C1A-C2A-CAA-CBA
18	A	813	CLA	C1A-C2A-CAA-CBA
18	A	841	CLA	C1A-C2A-CAA-CBA
18	B	830	CLA	C1A-C2A-CAA-CBA
18	B	833	CLA	C1A-C2A-CAA-CBA
22	A	852	LHG	C31-C32-C33-C34
18	B	821	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
22	1	622	LHG	O9-C7-C8-C9
18	1	602	CLA	C2A-CAA-CBA-CGA
18	A	836	CLA	CBD-CGD-O2D-CED
18	A	838	CLA	C6-C7-C8-C10
18	B	833	CLA	CAA-CBA-CGA-O1A
18	1	614	CLA	CAA-CBA-CGA-O1A
18	4	603	CLA	CAA-CBA-CGA-O2A
18	B	825	CLA	C3-C5-C6-C7
18	A	807	CLA	CAA-CBA-CGA-O1A
18	A	821	CLA	C2-C3-C5-C6
18	4	609	CLA	C4B-C3B-CAB-CBB
18	A	803	CLA	C4B-C3B-CAB-CBB
18	B	820	CLA	C4B-C3B-CAB-CBB
18	A	841	CLA	C16-C17-C18-C20
25	A	844	PQN	C26-C27-C28-C29
18	2	602	CLA	CAA-CBA-CGA-O1A
22	1	618	LHG	O9-C7-C8-C9
23	4	621	LMG	O7-C10-C11-C12
22	1	621	LHG	C32-C33-C34-C35
19	1	615	LUT	C1-C6-C7-C8
21	B	846	BCR	C23-C24-C25-C26
21	J	101	BCR	C5-C6-C7-C8
18	2	604	CLA	C13-C15-C16-C17
18	2	609	CLA	CAA-CBA-CGA-O1A
23	4	619	LMG	O8-C28-C29-C30
17	4	606	CHL	CAA-CBA-CGA-O1A
18	A	802	CLA	C16-C17-C18-C19
18	A	841	CLA	C16-C17-C18-C19
18	A	819	CLA	C2A-CAA-CBA-CGA
18	A	833	CLA	CAA-CBA-CGA-O1A
18	2	609	CLA	CAA-CBA-CGA-O2A
18	B	804	CLA	CAA-CBA-CGA-O1A
18	B	819	CLA	CAA-CBA-CGA-O1A
23	1	623	LMG	C15-C16-C17-C18
18	2	602	CLA	CAD-CBD-CGD-O1D
18	2	612	CLA	CAD-CBD-CGD-O1D
18	2	613	CLA	CAD-CBD-CGD-O1D
18	3	609	CLA	CAD-CBD-CGD-O1D
18	4	610	CLA	CAD-CBD-CGD-O1D
18	A	831	CLA	CAD-CBD-CGD-O1D
18	A	833	CLA	CAD-CBD-CGD-O1D
18	A	854	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
18	B	814	CLA	CAD-CBD-CGD-O1D
18	G	203	CLA	CAD-CBD-CGD-O1D
18	4	612	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	C10-C11-C12-C13
18	2	604	CLA	C11-C12-C13-C14
18	A	841	CLA	C14-C13-C15-C16
18	B	825	CLA	C11-C10-C8-C9
18	B	838	CLA	C11-C12-C13-C14
18	B	829	CLA	CBD-CGD-O2D-CED
18	A	834	CLA	C13-C15-C16-C17
18	2	602	CLA	CAA-CBA-CGA-O2A
18	A	833	CLA	CAA-CBA-CGA-O2A
22	1	621	LHG	O7-C7-C8-C9
18	B	826	CLA	CAA-CBA-CGA-O2A
18	H	201	CLA	CAA-CBA-CGA-O2A
22	2	617	LHG	O7-C7-C8-C9
23	1	620	LMG	C29-C30-C31-C32
18	A	809	CLA	C3-C5-C6-C7
18	A	821	CLA	C4-C3-C5-C6
18	B	810	CLA	C4-C3-C5-C6
18	B	823	CLA	C4-C3-C5-C6
22	1	621	LHG	C33-C34-C35-C36
18	1	608	CLA	C6-C7-C8-C10
18	1	608	CLA	C12-C13-C15-C16
18	1	609	CLA	C2-C3-C5-C6
18	2	603	CLA	CHA-CBD-CGD-O1D
18	3	606	CLA	C3A-C2A-CAA-CBA
18	3	606	CLA	CHA-CBD-CGD-O1D
18	3	611	CLA	CHA-CBD-CGD-O1D
18	3	611	CLA	CAD-CBD-CGD-O2D
18	A	817	CLA	C11-C10-C8-C7
18	A	821	CLA	C6-C7-C8-C10
18	A	828	CLA	C12-C13-C15-C16
18	A	830	CLA	C6-C7-C8-C10
18	B	802	CLA	C11-C12-C13-C15
18	B	809	CLA	C6-C7-C8-C10
18	B	821	CLA	C3A-C2A-CAA-CBA
18	B	822	CLA	C6-C7-C8-C10
18	B	833	CLA	C6-C7-C8-C10
18	B	838	CLA	C11-C12-C13-C15
18	L	303	CLA	C11-C10-C8-C7
18	1	602	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
21	A	847	BCR	C7-C8-C9-C10
21	B	846	BCR	C21-C22-C23-C24
21	J	101	BCR	C21-C22-C23-C24
21	K	204	BCR	C21-C22-C23-C24
21	L	301	BCR	C11-C12-C13-C14
22	1	621	LHG	O9-C7-C8-C9
23	4	621	LMG	O9-C10-C11-C12
18	G	202	CLA	CAA-CBA-CGA-O2A
18	A	821	CLA	CAA-CBA-CGA-O2A
22	1	618	LHG	C24-C25-C26-C27
22	A	852	LHG	C27-C28-C29-C30
18	B	819	CLA	CAA-CBA-CGA-O2A
18	A	807	CLA	C15-C16-C17-C18
18	A	821	CLA	CAA-CBA-CGA-O1A
18	B	840	CLA	CAA-CBA-CGA-O1A
23	4	619	LMG	O10-C28-C29-C30
18	K	202	CLA	CBD-CGD-O2D-CED
18	1	611	CLA	C2A-CAA-CBA-CGA
18	A	808	CLA	C2A-CAA-CBA-CGA
18	B	822	CLA	C11-C12-C13-C15
18	B	822	CLA	CAA-CBA-CGA-O1A
18	L	303	CLA	C4-C3-C5-C6
17	1	601	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

124 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	F	301	CLA	1	0
21	B	846	BCR	1	0
18	B	812	CLA	3	0
18	1	608	CLA	1	0
18	B	825	CLA	1	0
18	H	201	CLA	3	0
21	K	204	BCR	3	0
22	2	617	LHG	3	0
19	3	614	LUT	4	0
18	A	836	CLA	1	0
18	A	806	CLA	1	0
19	1	615	LUT	3	0
17	2	606	CHL	1	0
18	1	603	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	4	614	CLA	1	0
18	A	817	CLA	4	0
21	A	846	BCR	2	0
22	A	855	LHG	3	0
21	A	850	BCR	5	0
18	B	829	CLA	2	0
21	L	306	BCR	2	0
21	A	845	BCR	3	0
18	B	840	CLA	3	0
18	4	602	CLA	2	0
18	B	826	CLA	3	0
18	A	842	CLA	1	0
23	1	620	LMG	1	0
18	3	602	CLA	1	0
17	4	606	CHL	2	0
18	1	613	CLA	1	0
18	A	804	CLA	1	0
17	2	614	CHL	1	0
18	2	604	CLA	1	0
18	A	828	CLA	1	0
19	1	619	LUT	5	0
20	3	615	XAT	3	0
21	J	103	BCR	2	0
21	1	617	BCR	1	0
21	A	849	BCR	3	0
18	A	810	CLA	2	0
18	1	612	CLA	2	0
18	K	202	CLA	3	0
23	1	623	LMG	1	0
17	4	607	CHL	1	0
18	A	832	CLA	1	0
18	J	102	CLA	1	0
18	A	841	CLA	1	0
18	A	831	CLA	1	0
18	B	839	CLA	3	0
18	A	834	CLA	1	0
18	B	801	CLA	1	0
21	F	305	BCR	1	0
18	A	854	CLA	2	0
23	F	306	LMG	1	0
18	B	813	CLA	2	0
18	A	809	CLA	2	0

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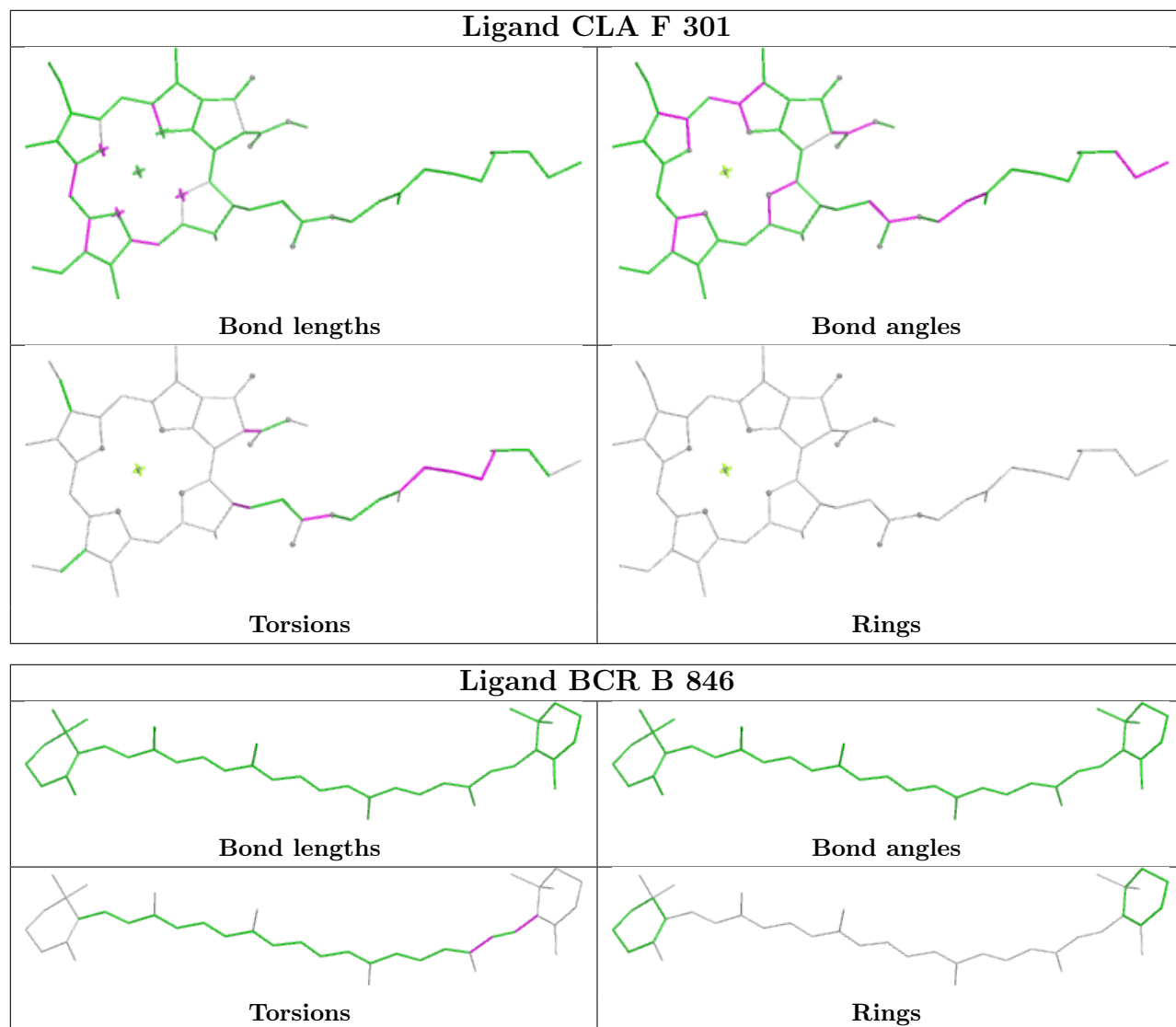
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	3	616	CHL	1	0
18	B	815	CLA	1	0
21	J	101	BCR	6	0
17	2	607	CHL	2	0
21	B	844	BCR	1	0
18	1	609	CLA	2	0
18	A	807	CLA	3	0
18	B	823	CLA	2	0
18	B	838	CLA	2	0
18	3	611	CLA	3	0
23	F	307	LMG	1	0
18	B	816	CLA	4	0
21	B	847	BCR	3	0
18	A	802	CLA	3	0
18	B	817	CLA	2	0
18	2	612	CLA	1	0
18	A	843	CLA	2	0
21	F	302	BCR	1	0
27	B	848	DGD	2	0
21	2	618	BCR	5	0
18	G	203	CLA	1	0
21	L	301	BCR	2	0
18	K	203	CLA	1	0
21	G	205	BCR	1	0
18	A	821	CLA	1	0
18	A	837	CLA	1	0
24	A	856	LMT	1	0
21	3	601	BCR	2	0
18	B	811	CLA	1	0
18	B	828	CLA	1	0
18	2	609	CLA	2	0
19	2	615	LUT	1	0
21	B	842	BCR	2	0
18	B	809	CLA	4	0
18	A	829	CLA	1	0
21	A	847	BCR	2	0
22	1	618	LHG	1	0
20	2	616	XAT	1	0
17	2	601	CHL	1	0
21	L	307	BCR	1	0
25	B	841	PQN	2	0
18	A	827	CLA	1	0

Continued on next page...

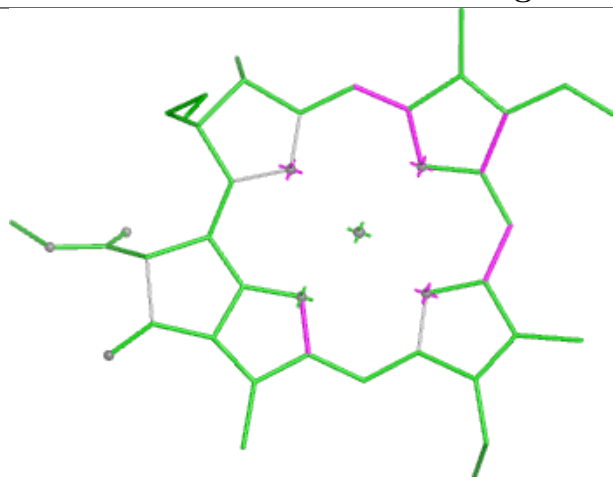
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	1	621	LHG	2	0
18	2	610	CLA	1	0
18	A	818	CLA	1	0
18	B	827	CLA	1	0
18	L	302	CLA	3	0
18	B	804	CLA	1	0
21	L	305	BCR	2	0
18	3	603	CLA	2	0
17	1	606	CHL	1	0
18	A	803	CLA	1	0
18	A	819	CLA	1	0
18	A	830	CLA	2	0
18	B	807	CLA	2	0
19	4	616	LUT	5	0
18	4	601	CLA	1	0
18	A	825	CLA	2	0
18	A	808	CLA	1	0
21	B	845	BCR	1	0
23	B	849	LMG	2	0
18	B	821	CLA	2	0
17	4	605	CHL	4	0
21	B	843	BCR	1	0
18	3	617	CLA	1	0
22	1	622	LHG	1	0
18	1	614	CLA	1	0
18	A	812	CLA	1	0

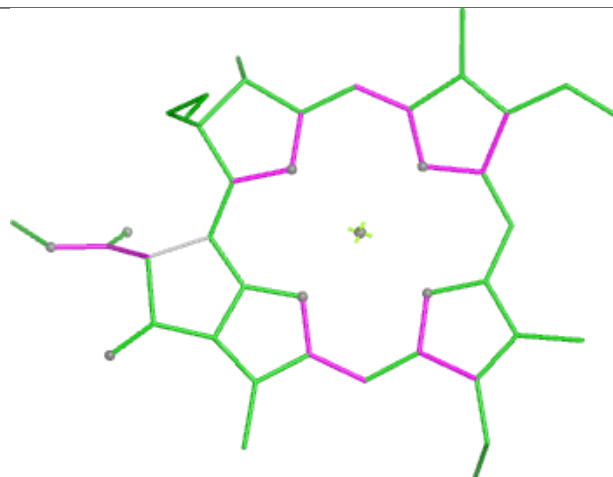
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



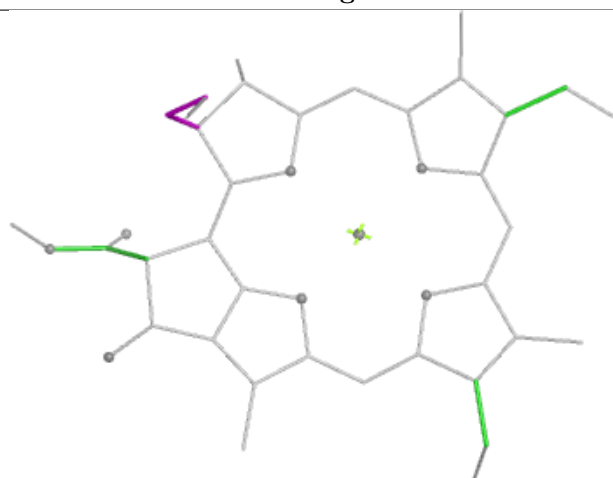
Ligand CLA B 830



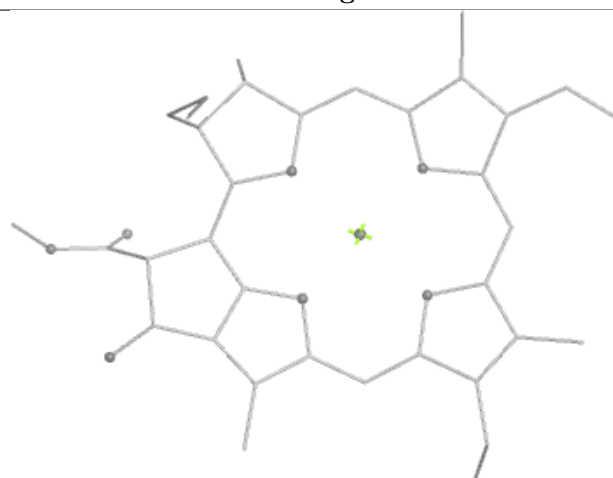
Bond lengths



Bond angles

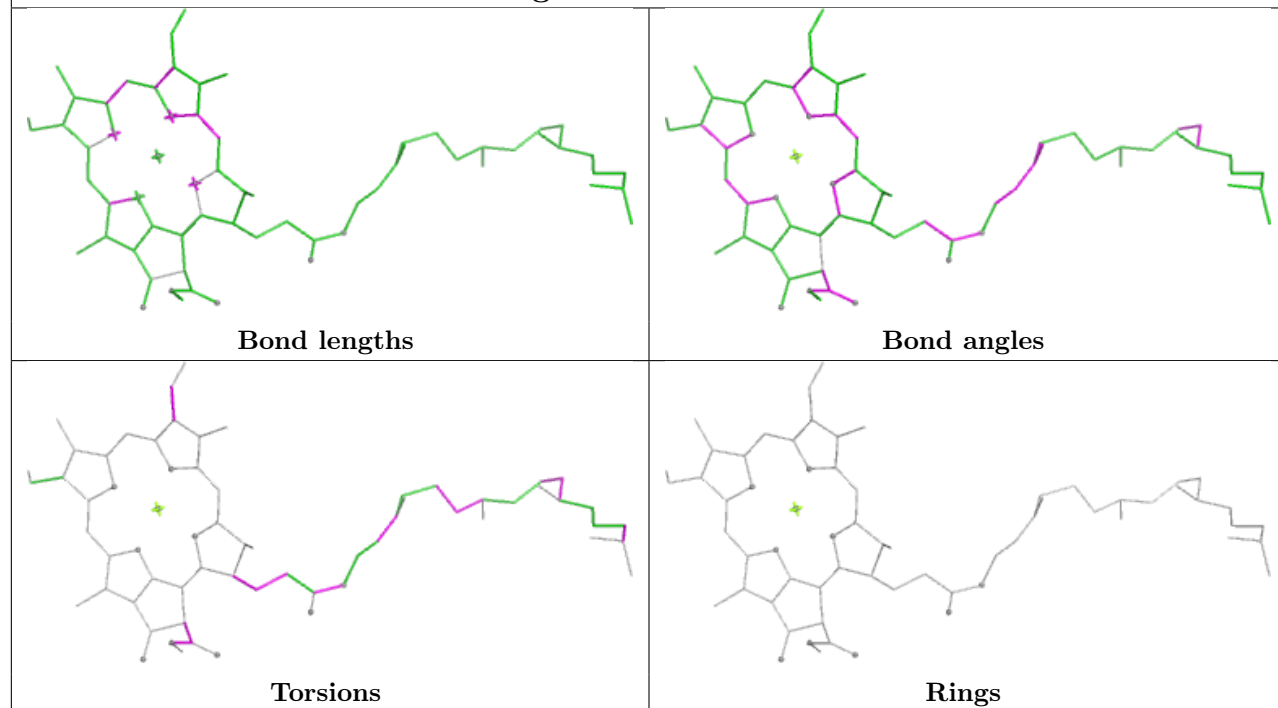


Torsions

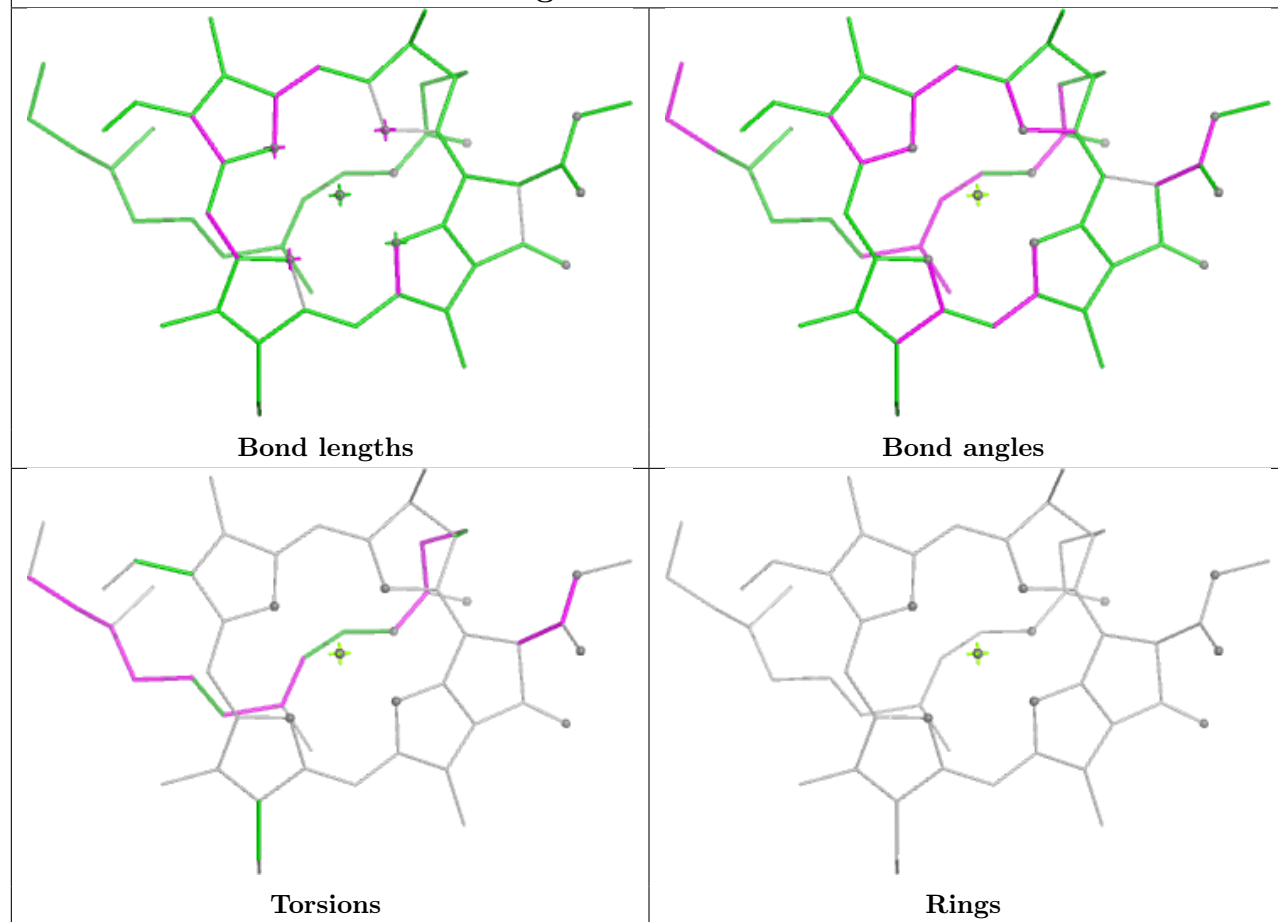


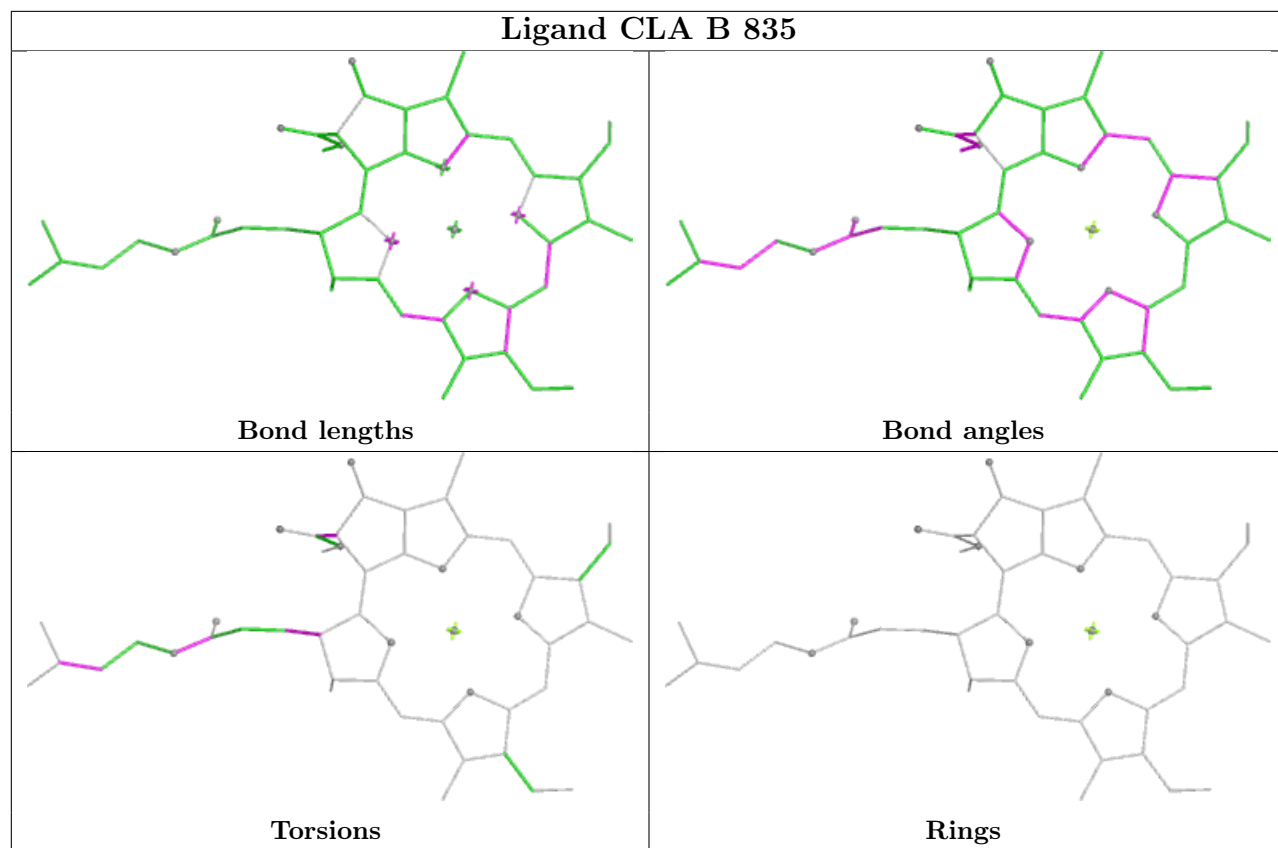
Rings

Ligand CLA B 812

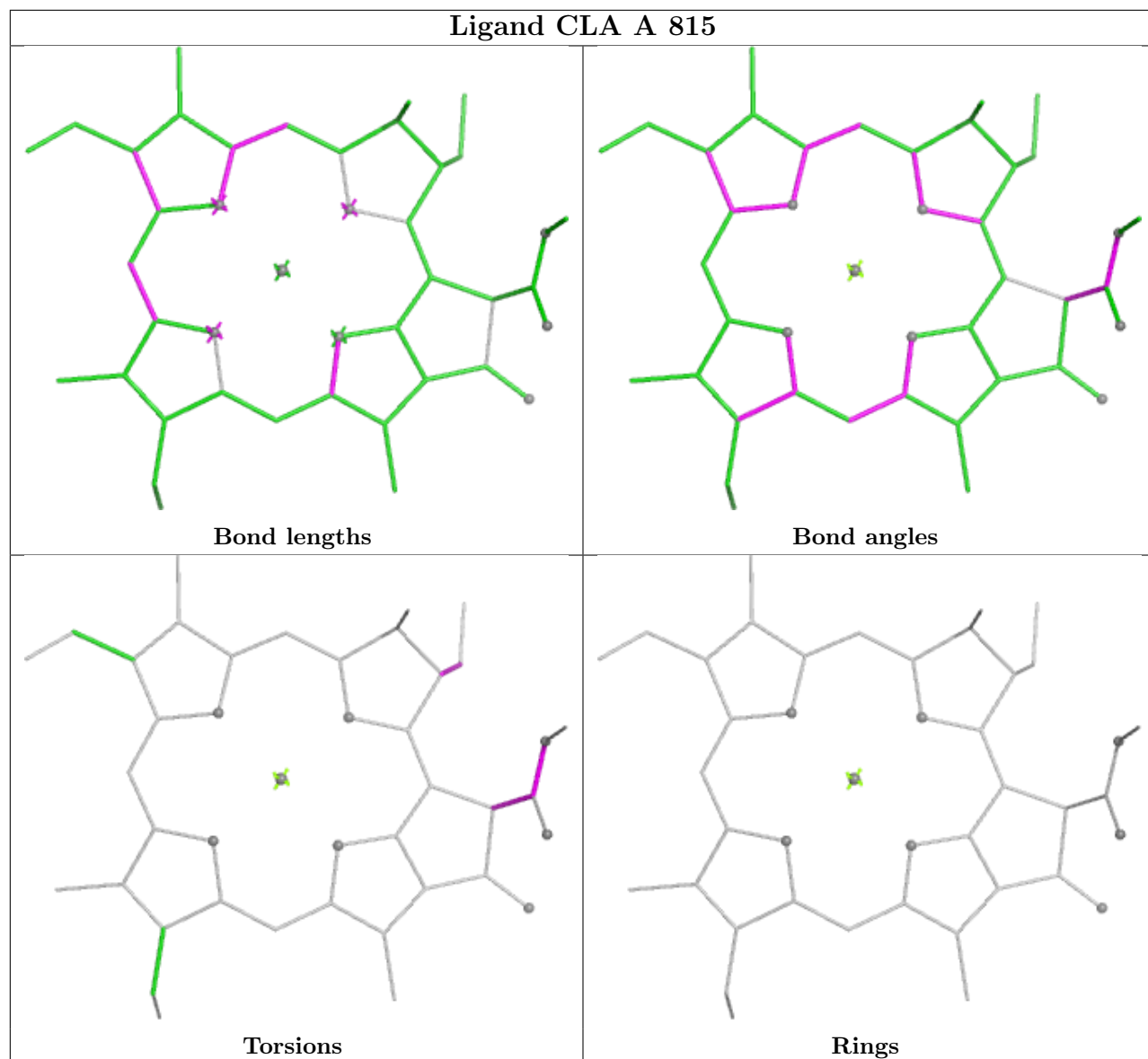


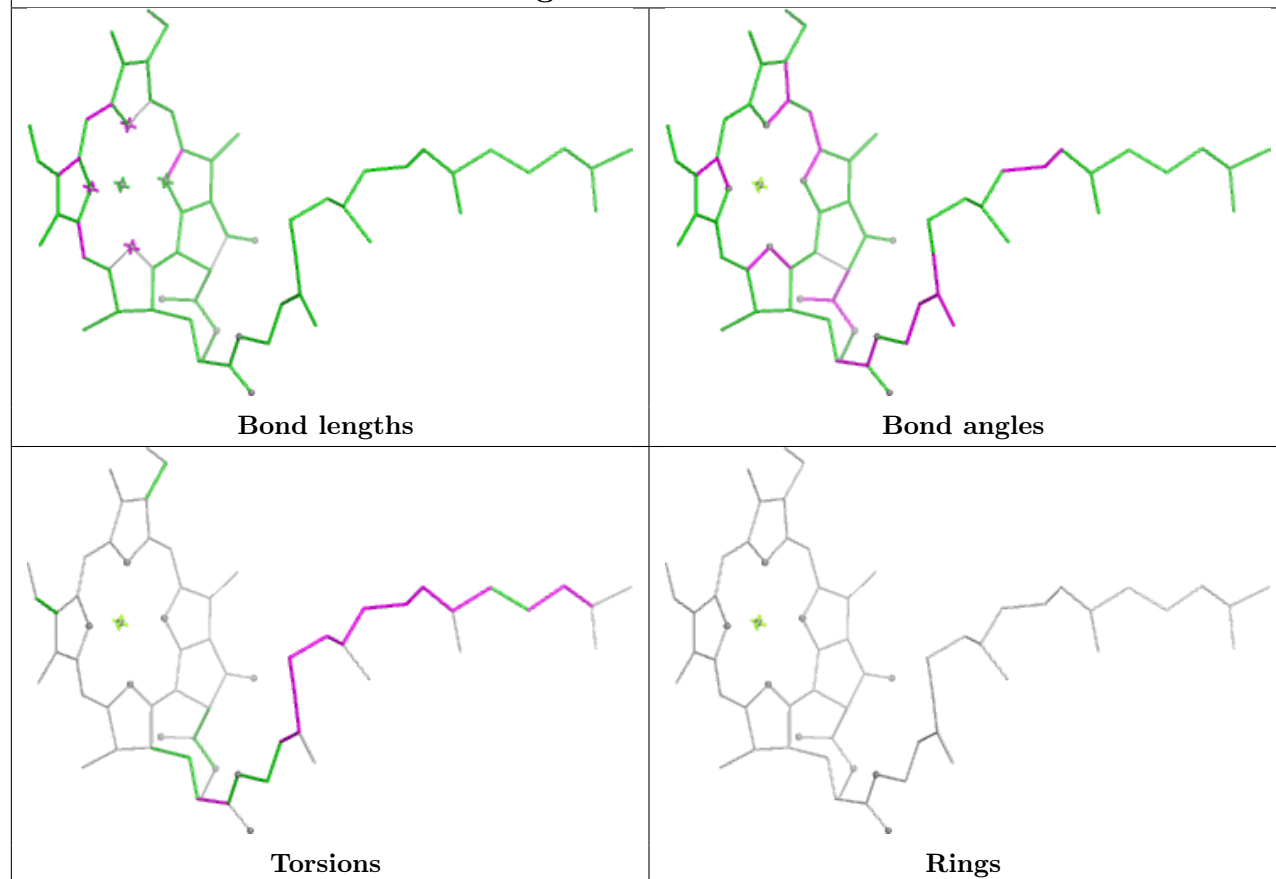
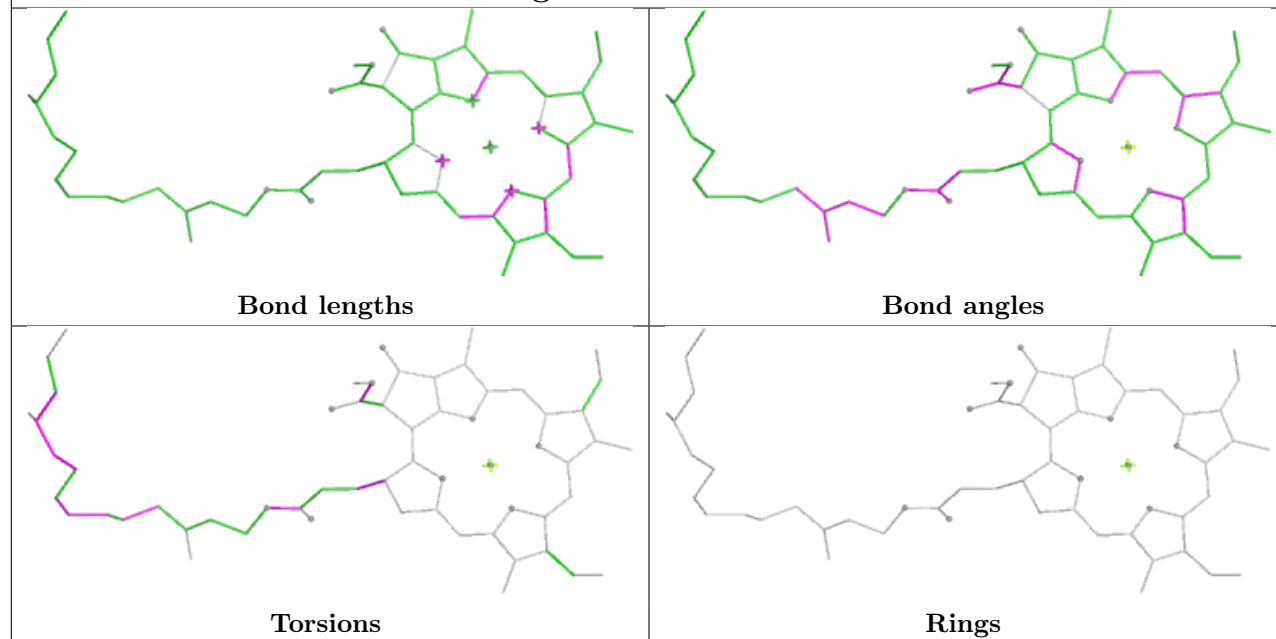
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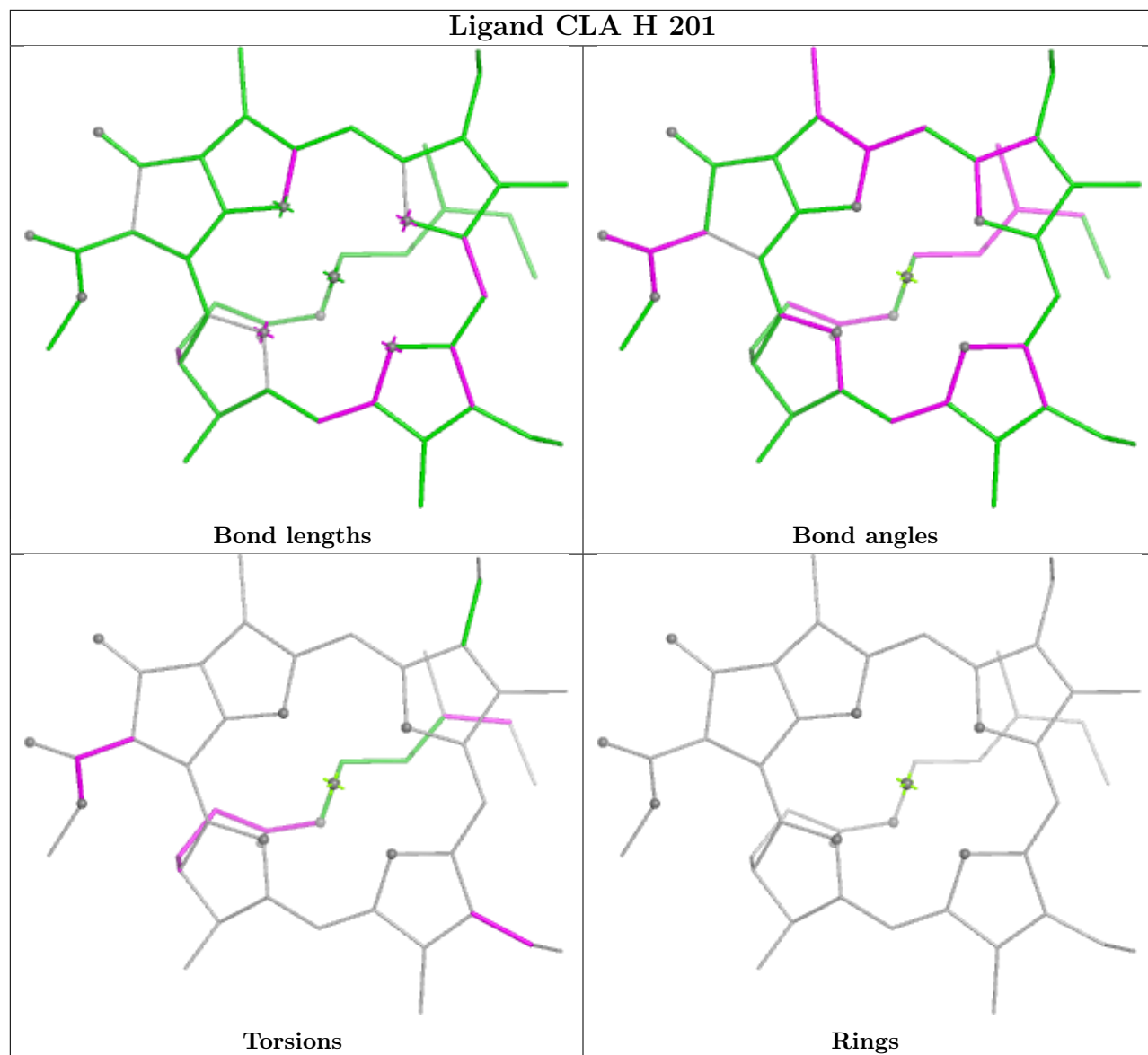




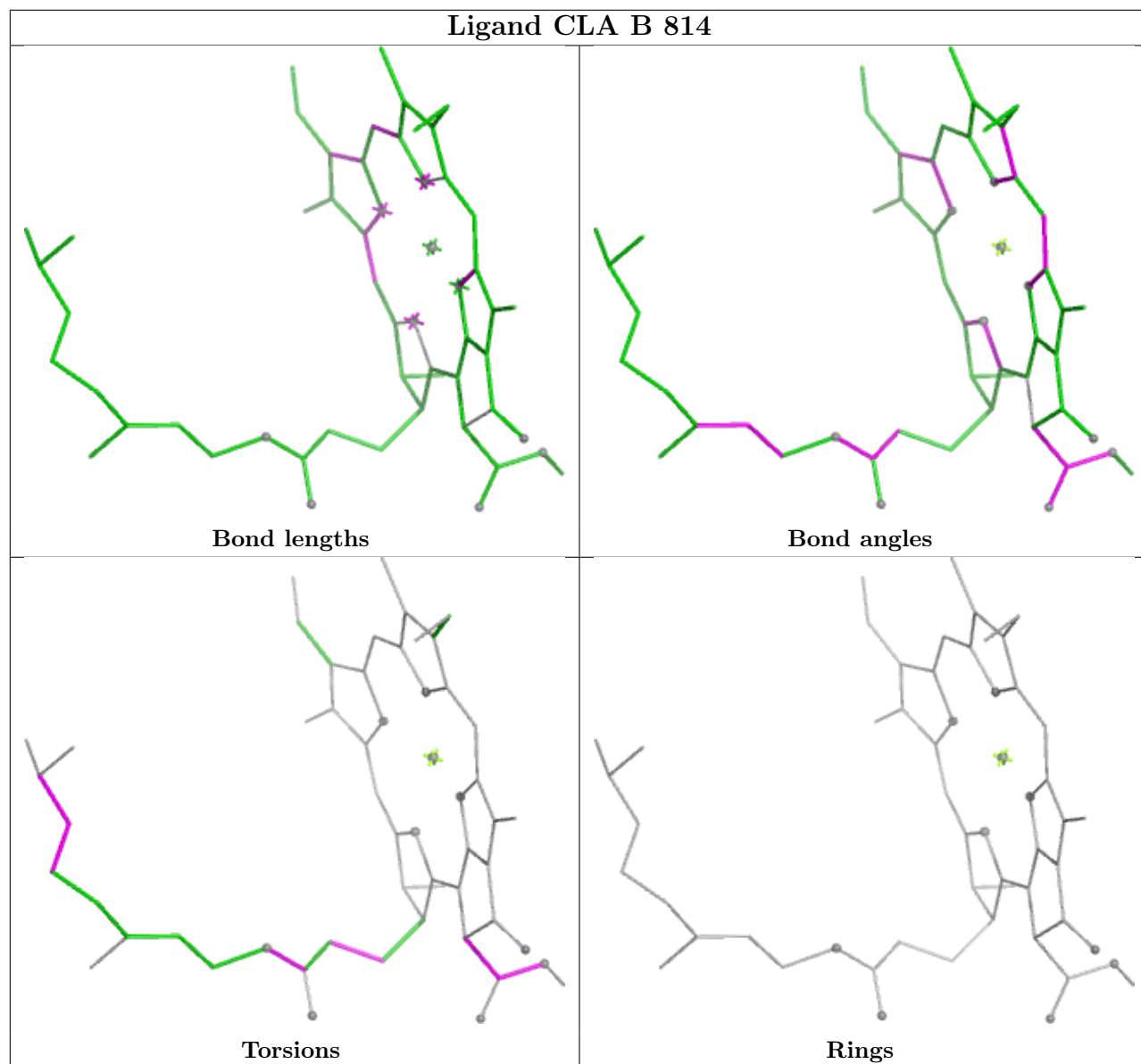
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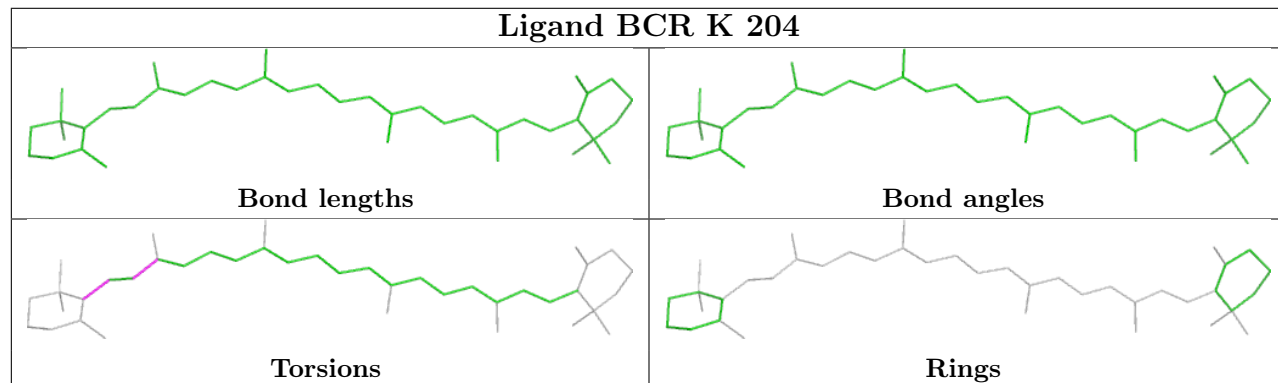
Ligand CLA 1 608**Ligand CLA B 825**

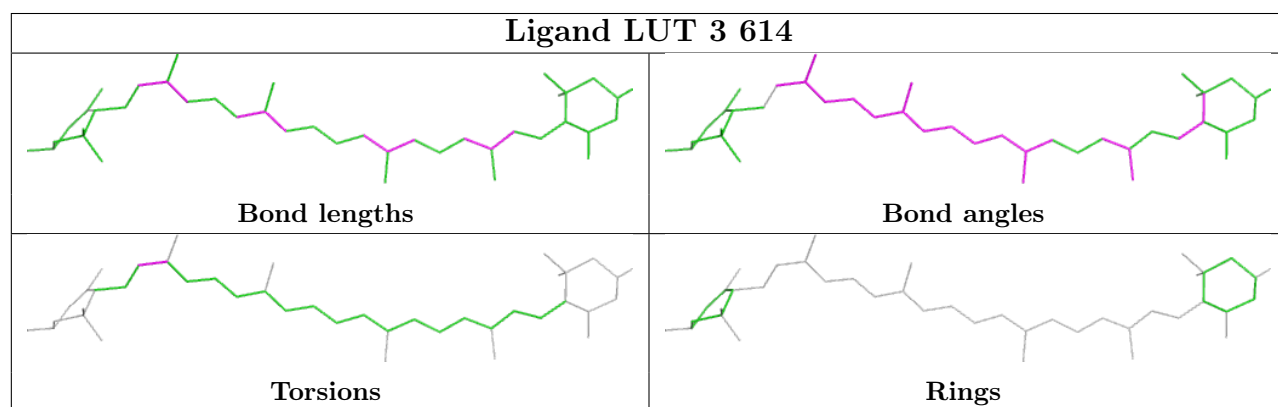
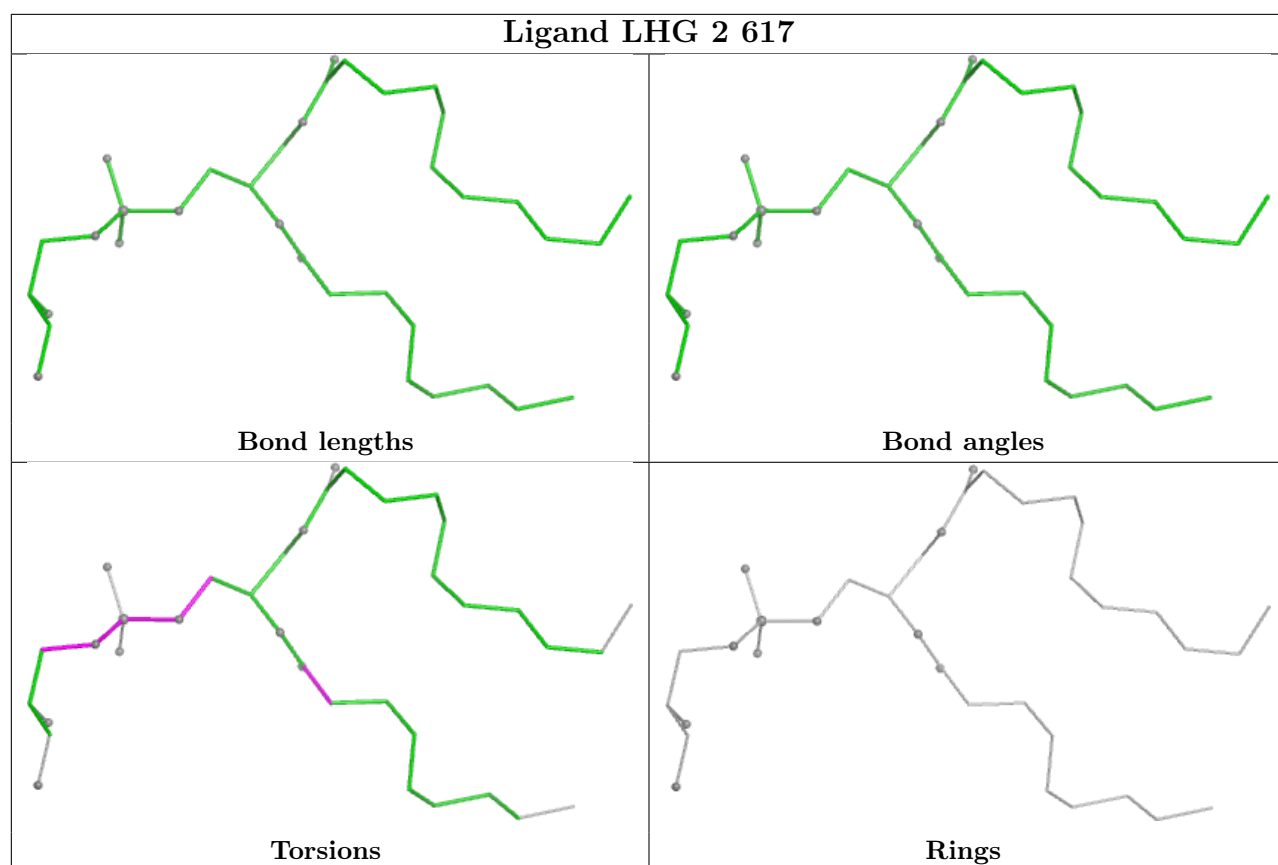


Ligand CLA B 814

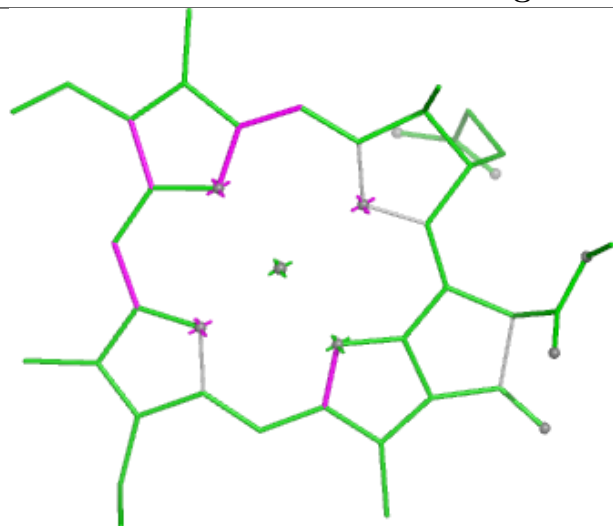


Ligand BCR K 204

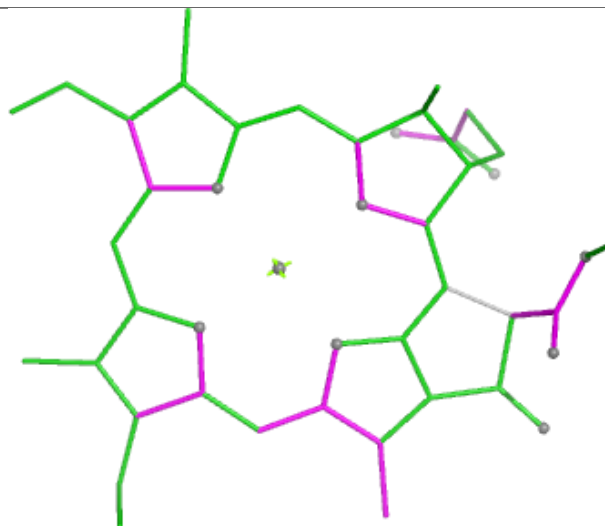




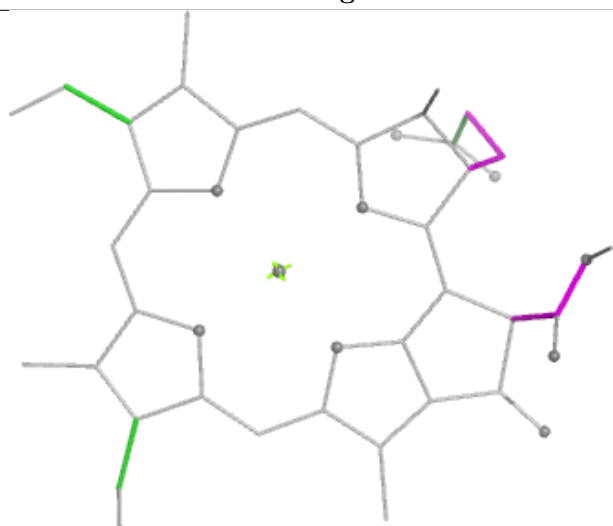
Ligand CLA A 836



Bond lengths



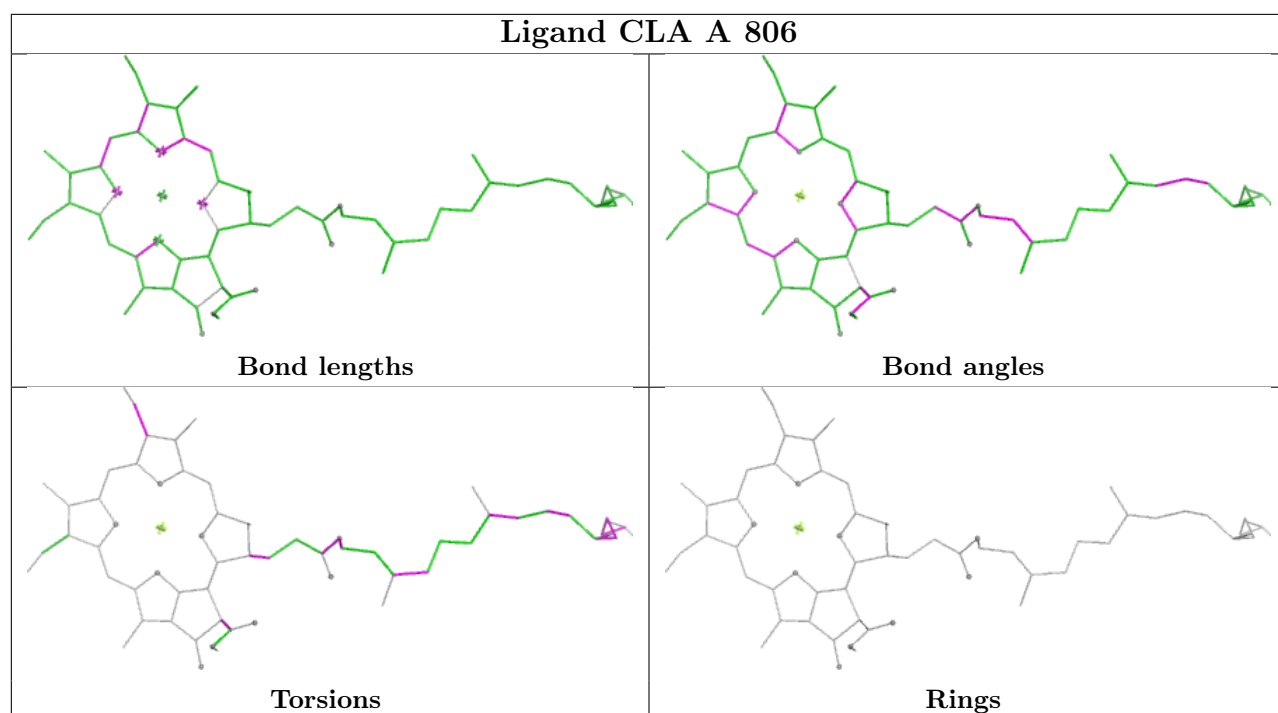
Bond angles



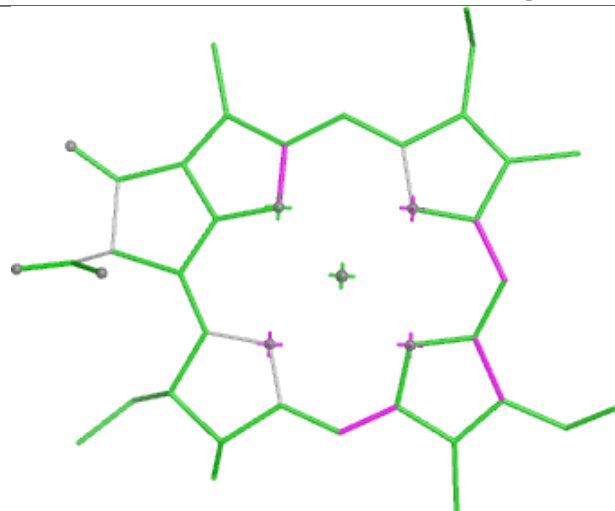
Torsions



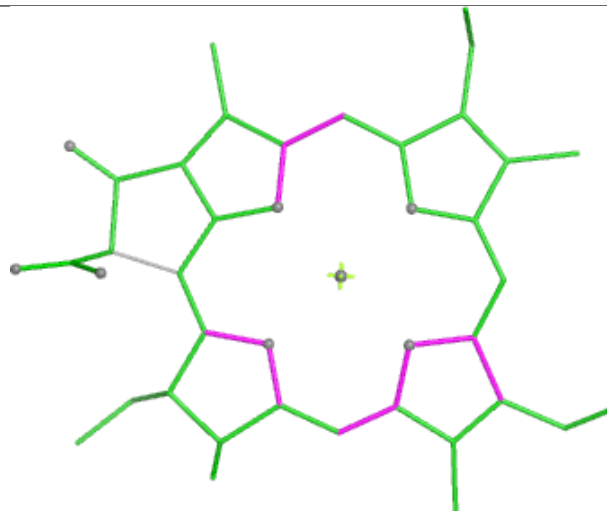
Rings



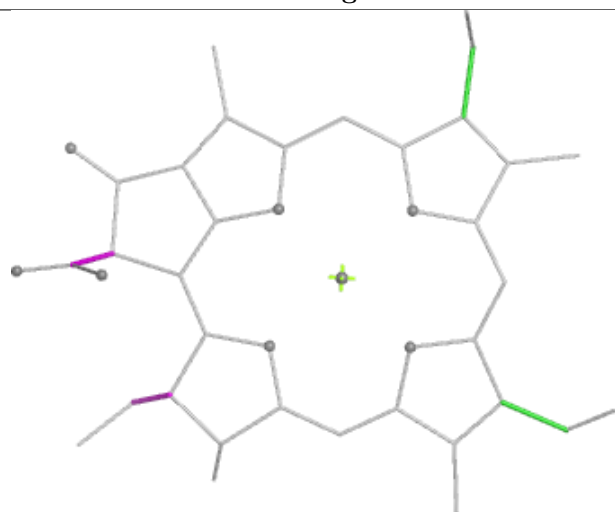
Ligand CLA 3 606



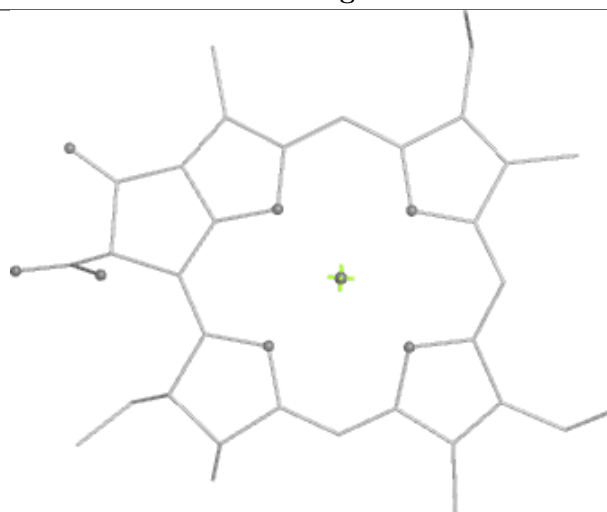
Bond lengths



Bond angles

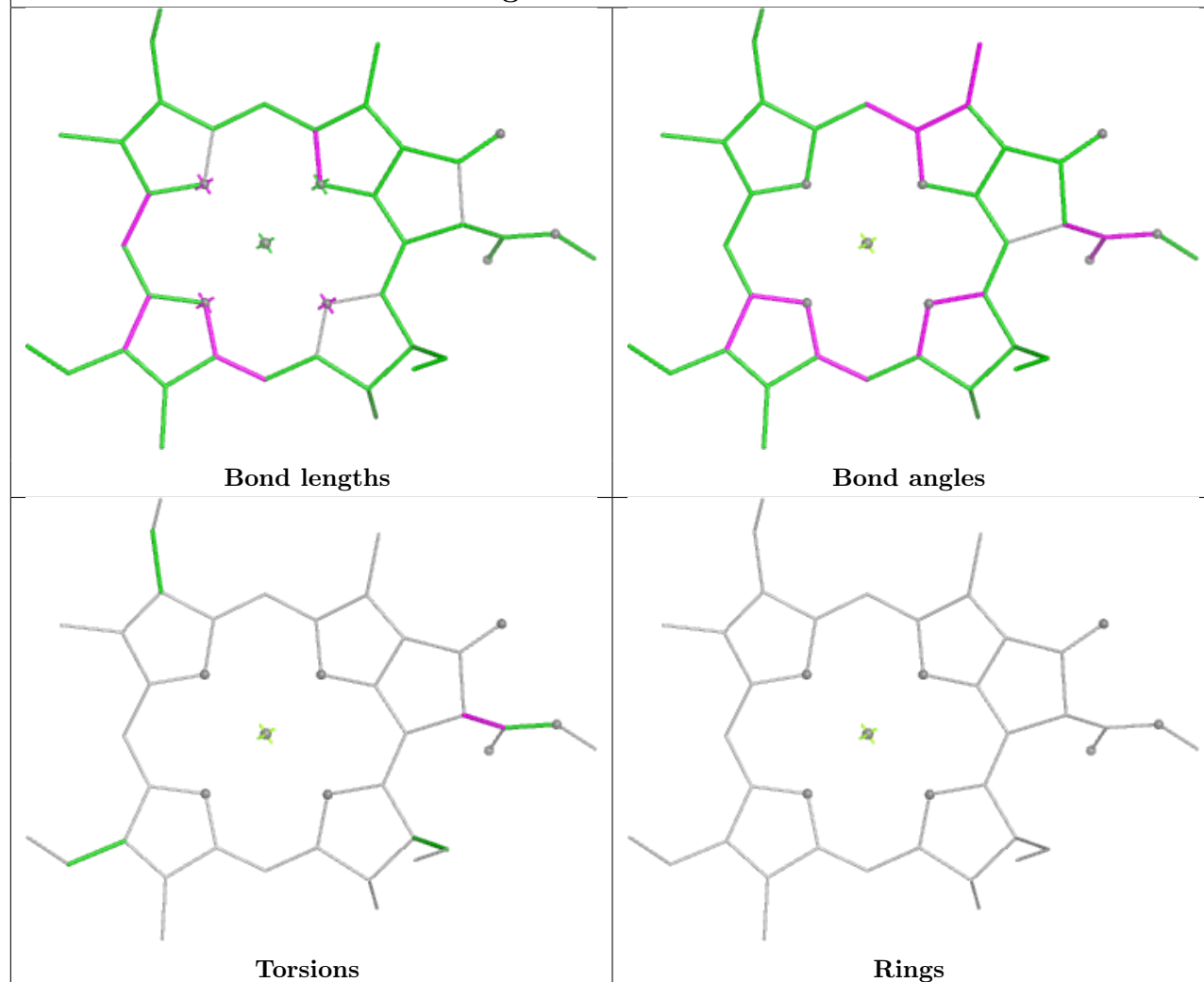


Torsions

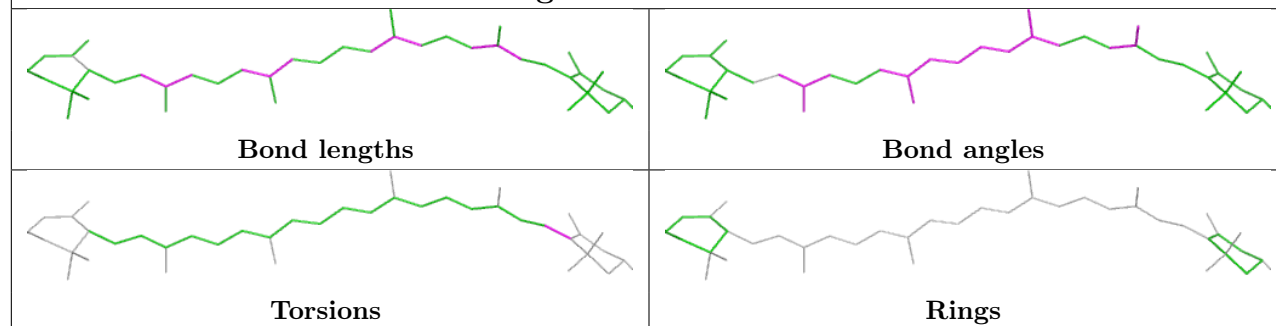


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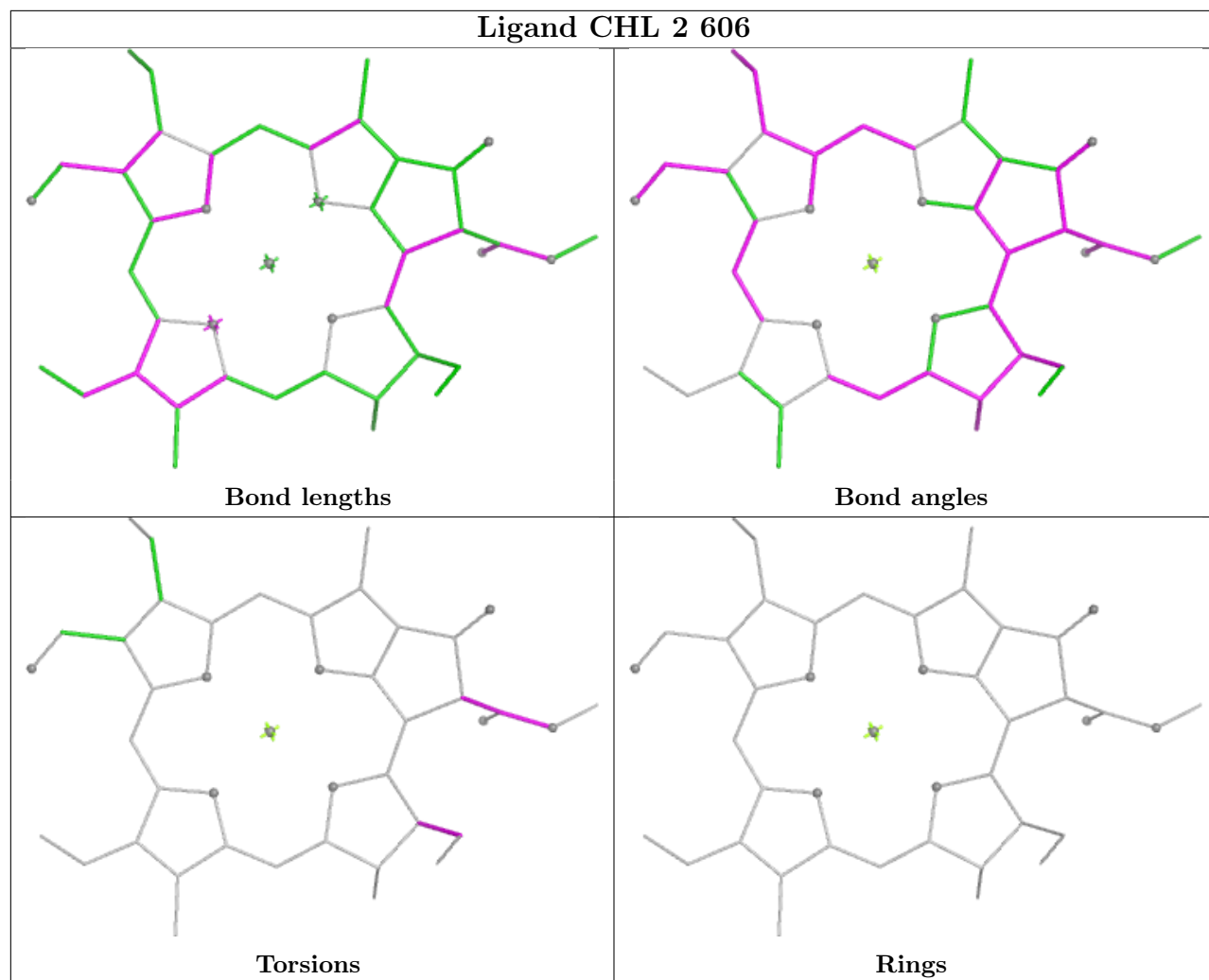
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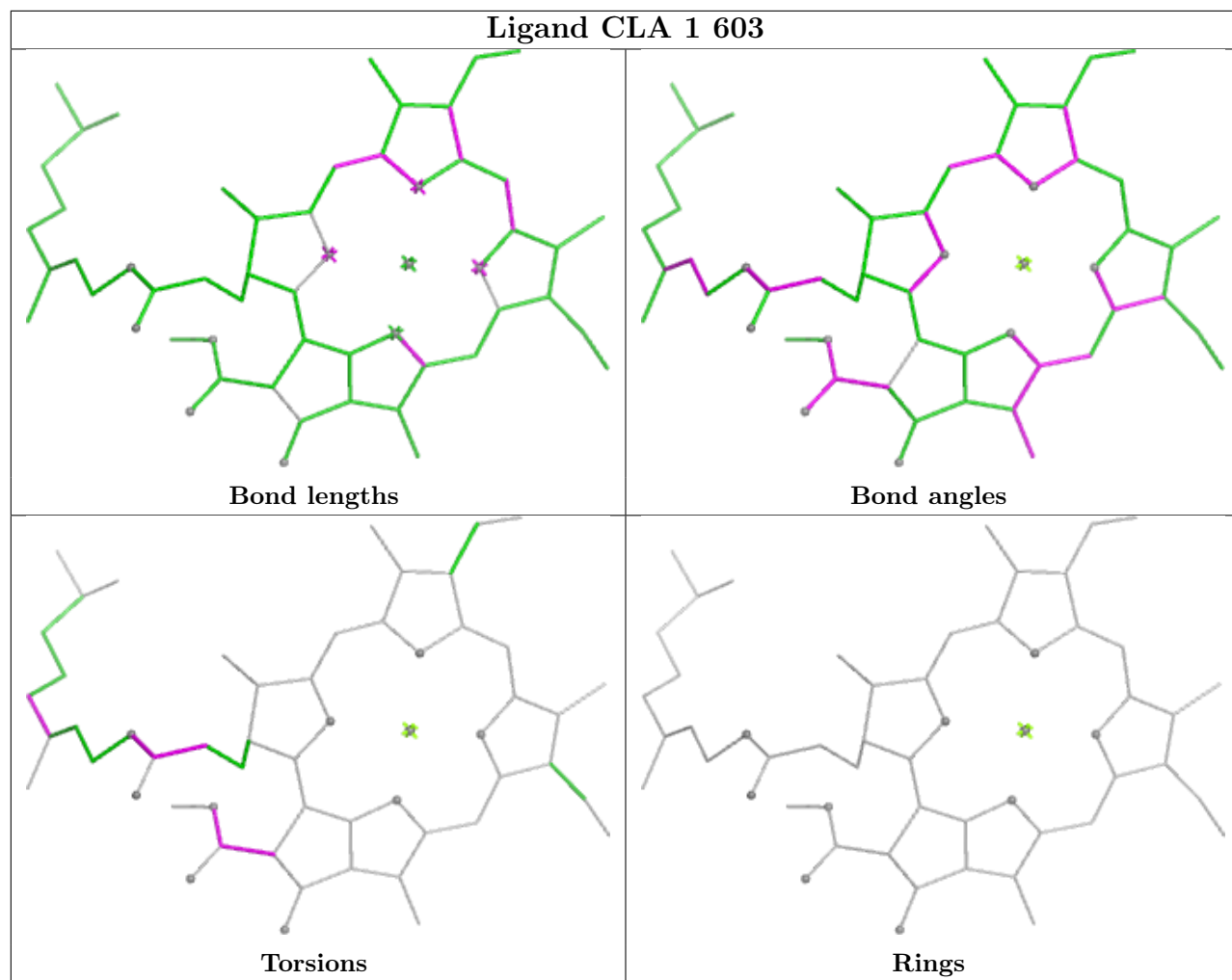


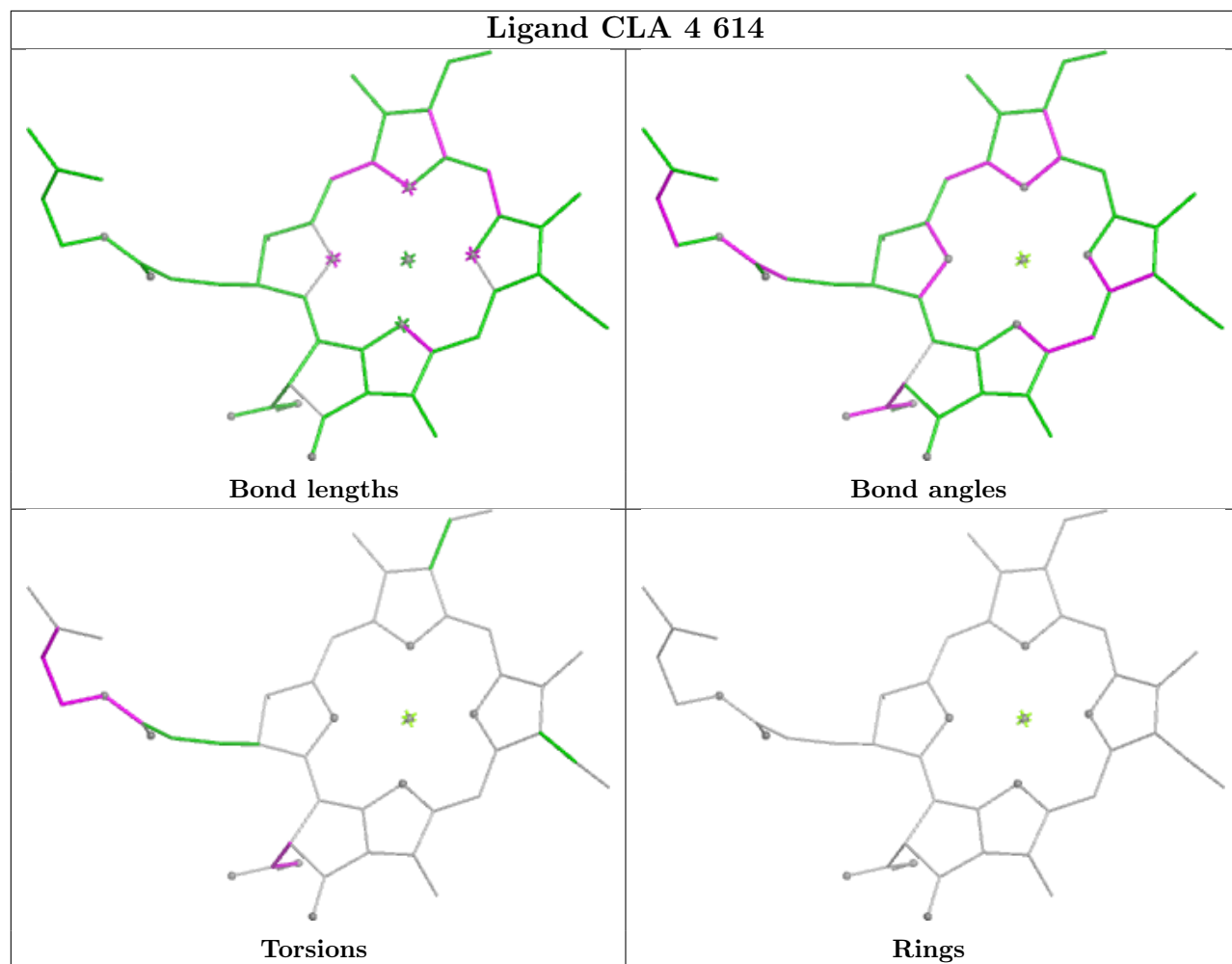
Ligand LUT 1 615



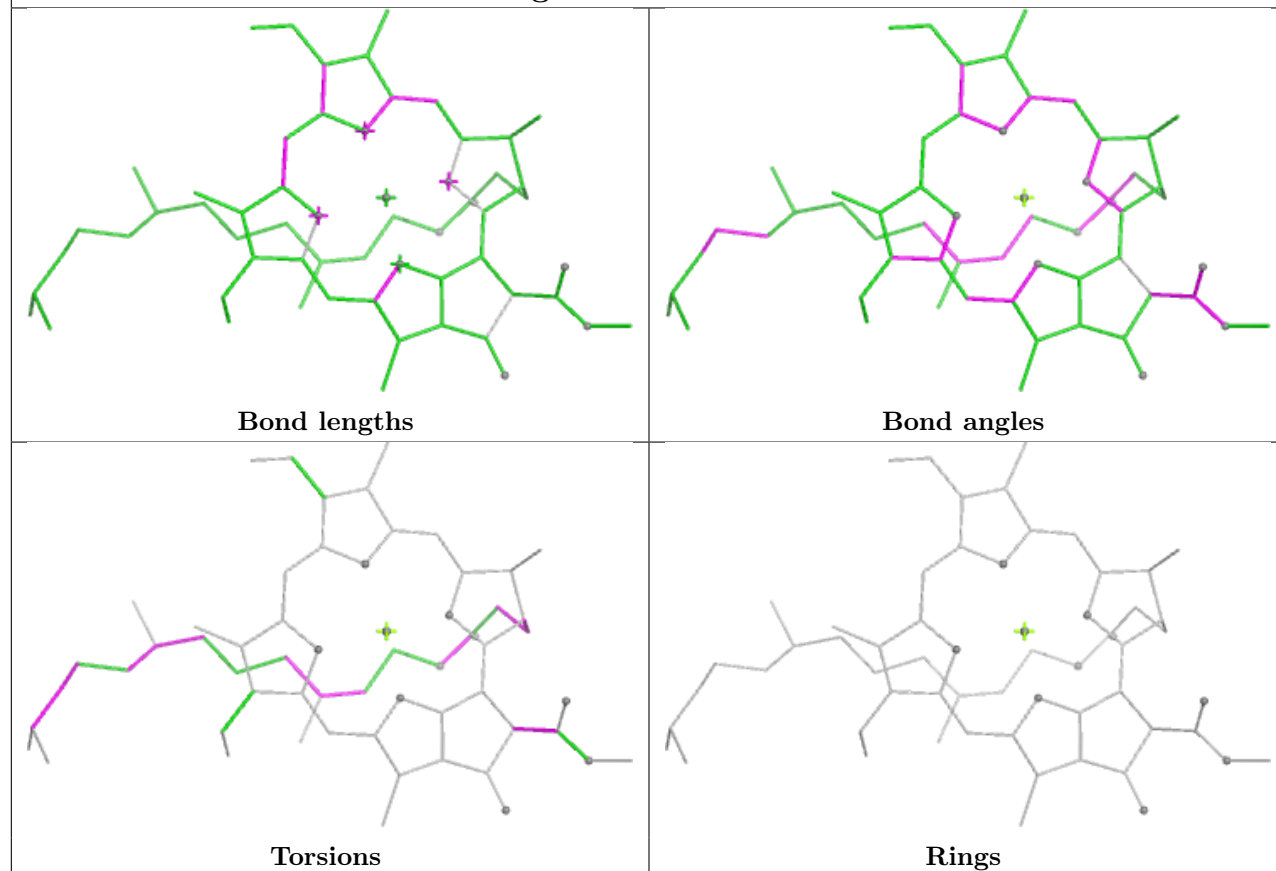
Ligand CHL 2 606



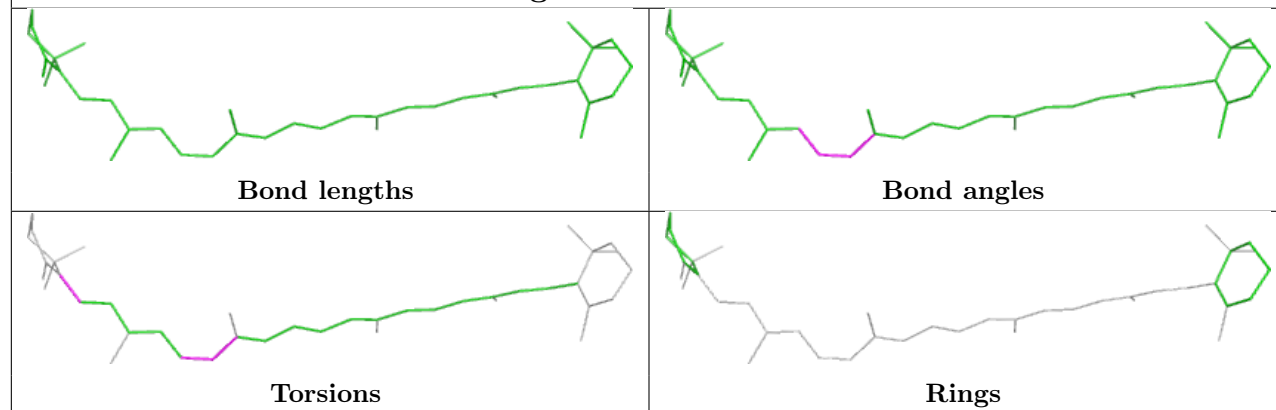


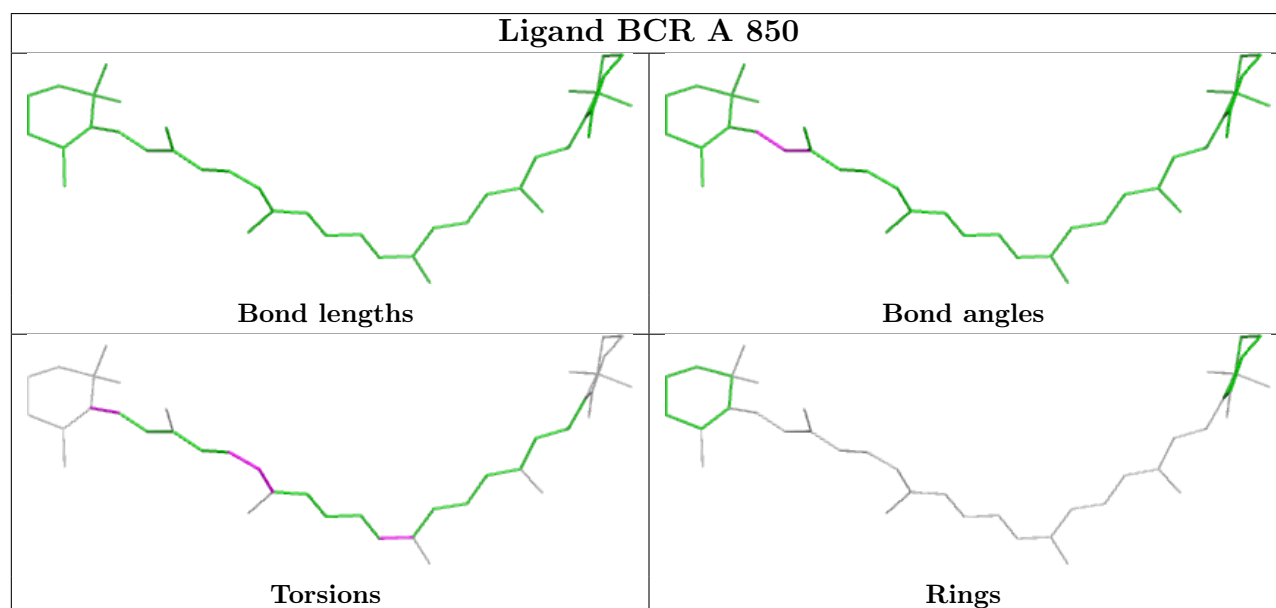
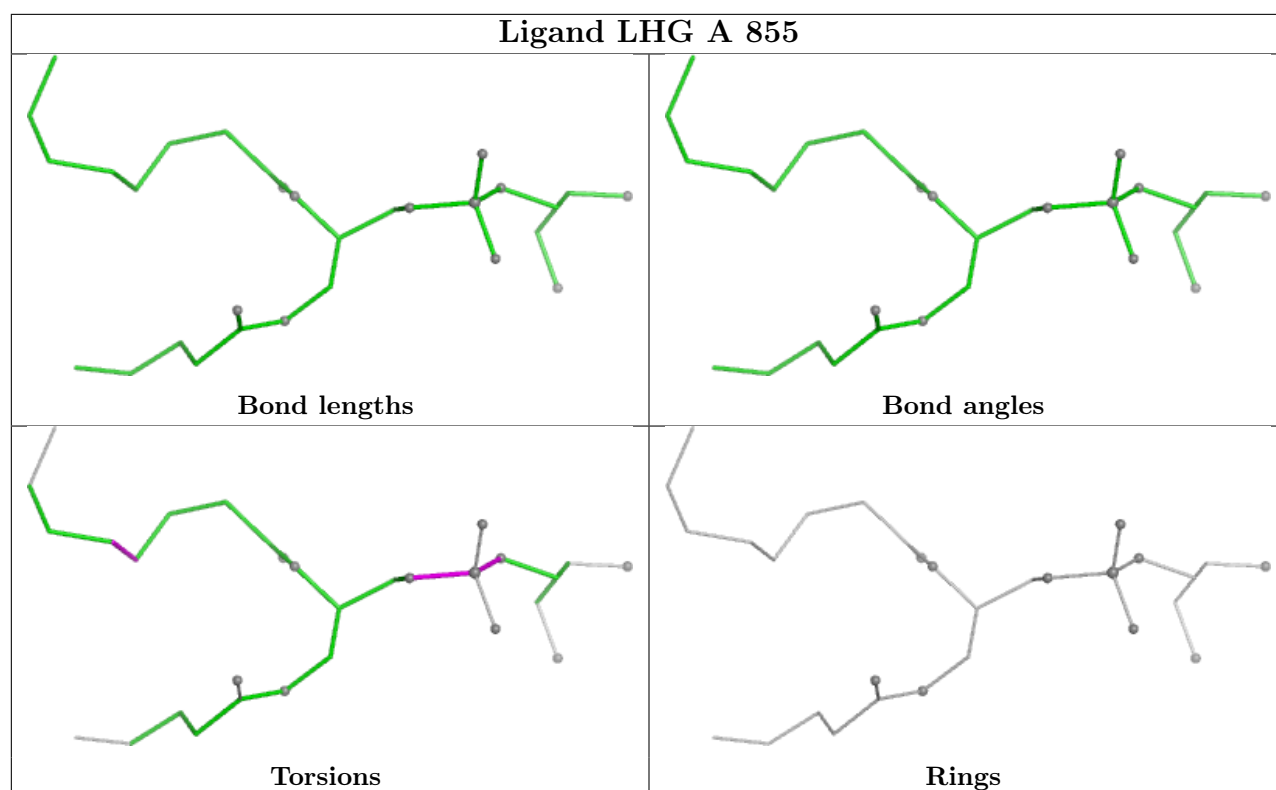


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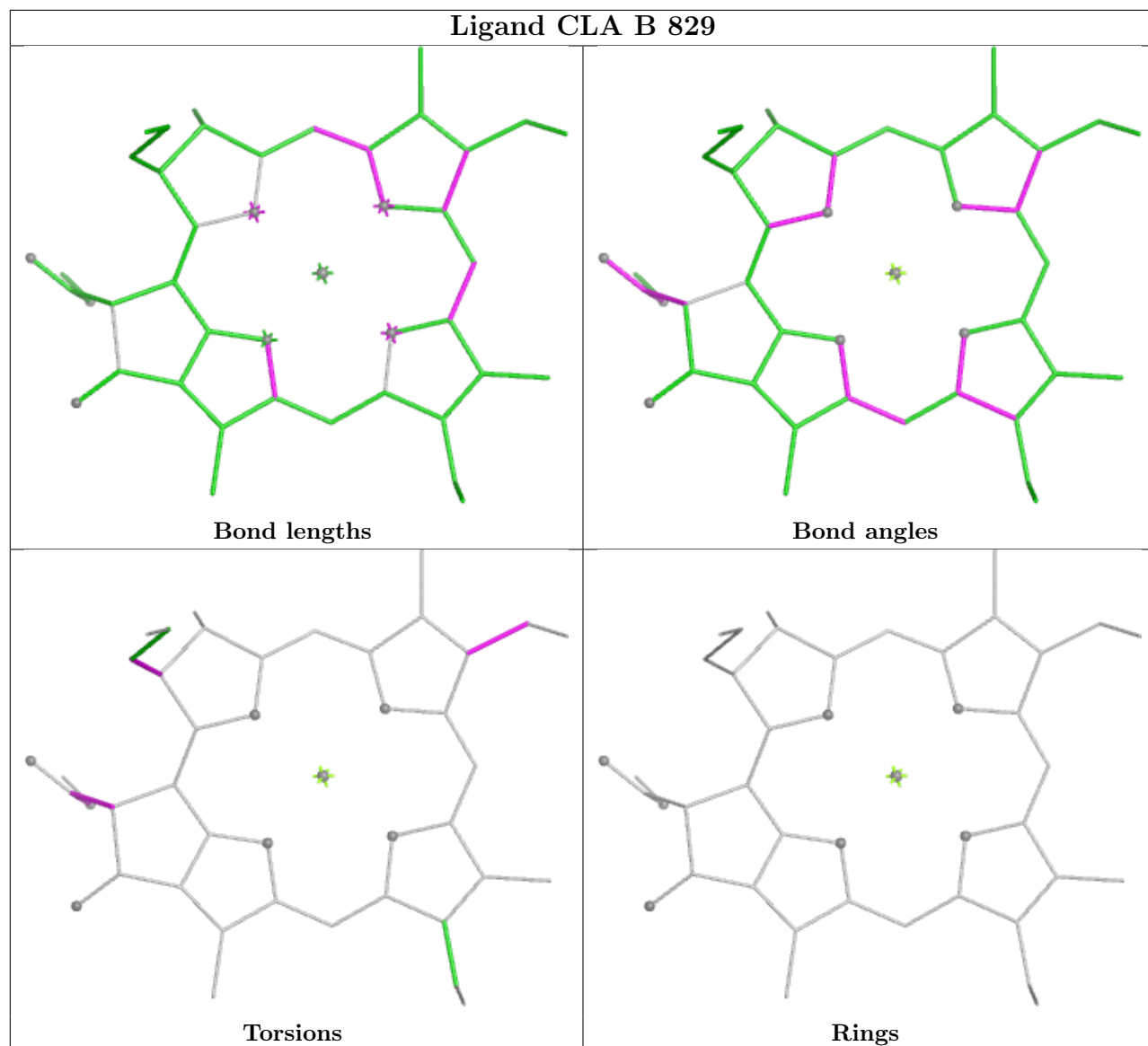


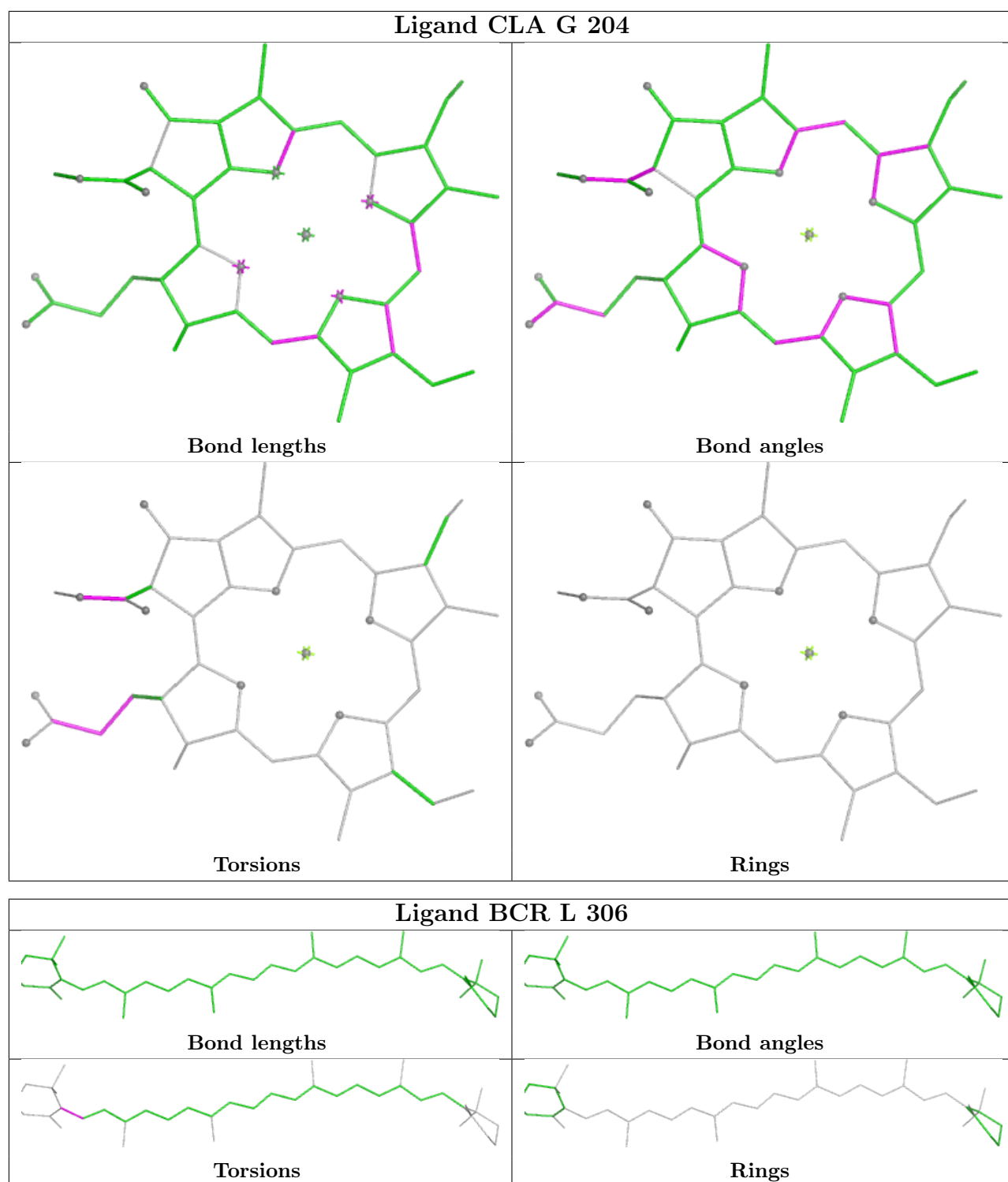
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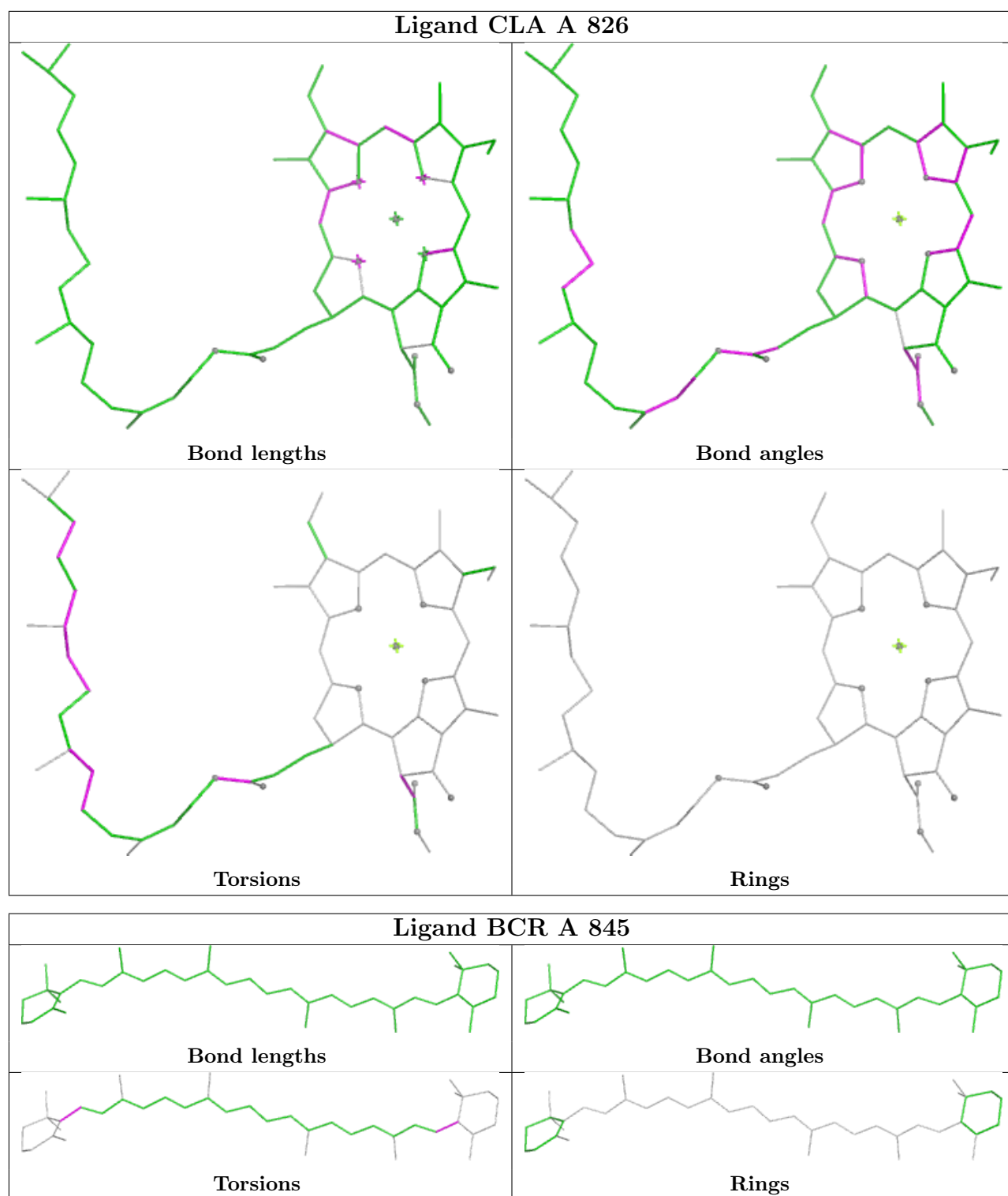


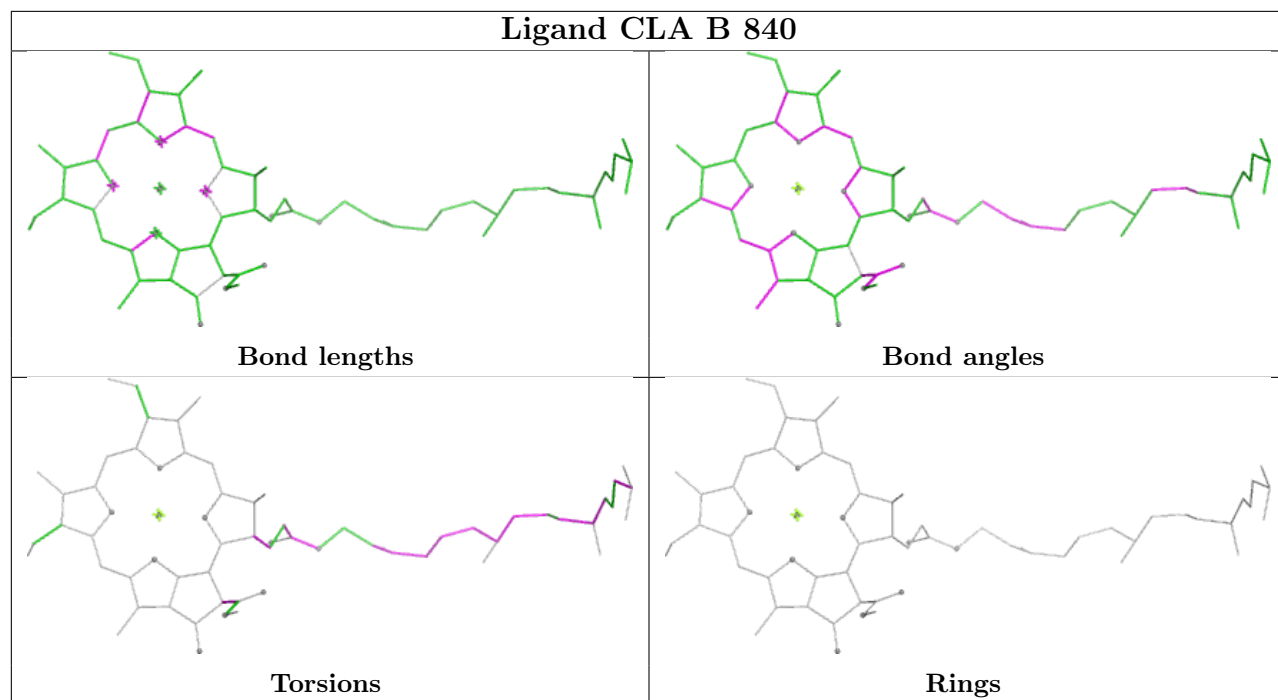


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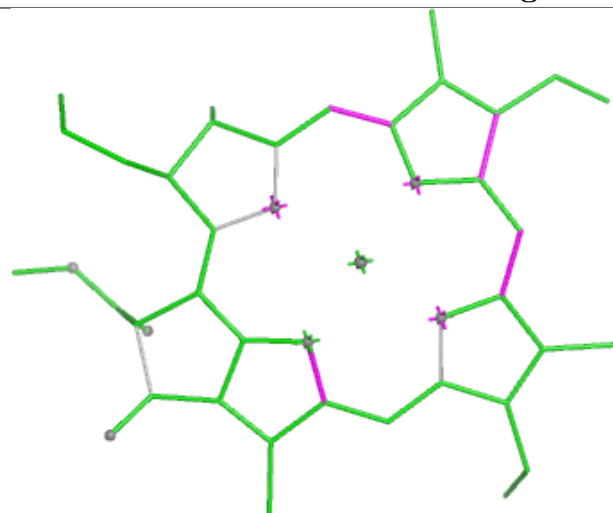




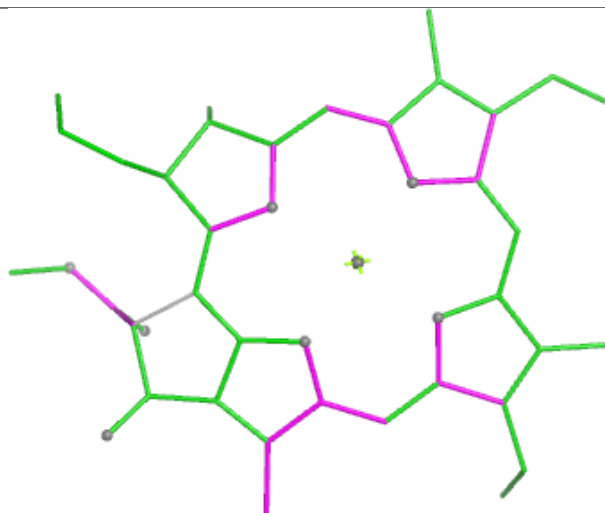




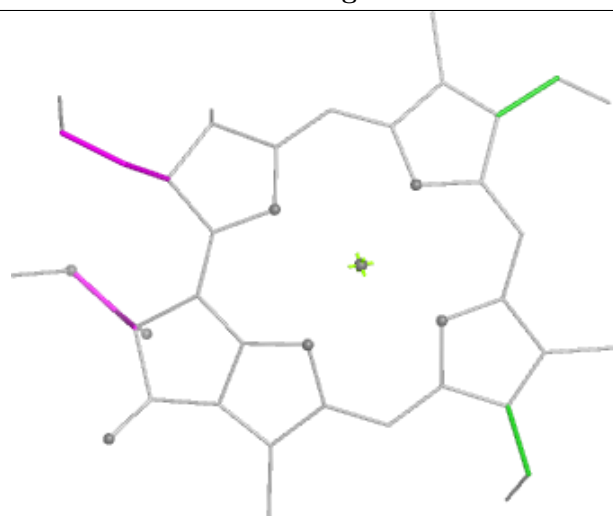
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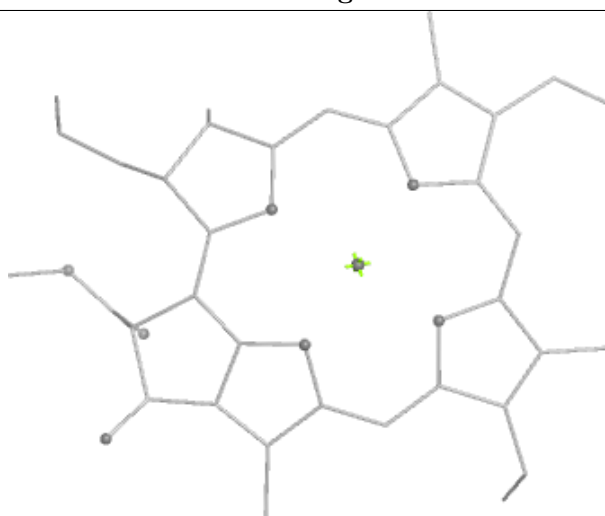
Bond lengths



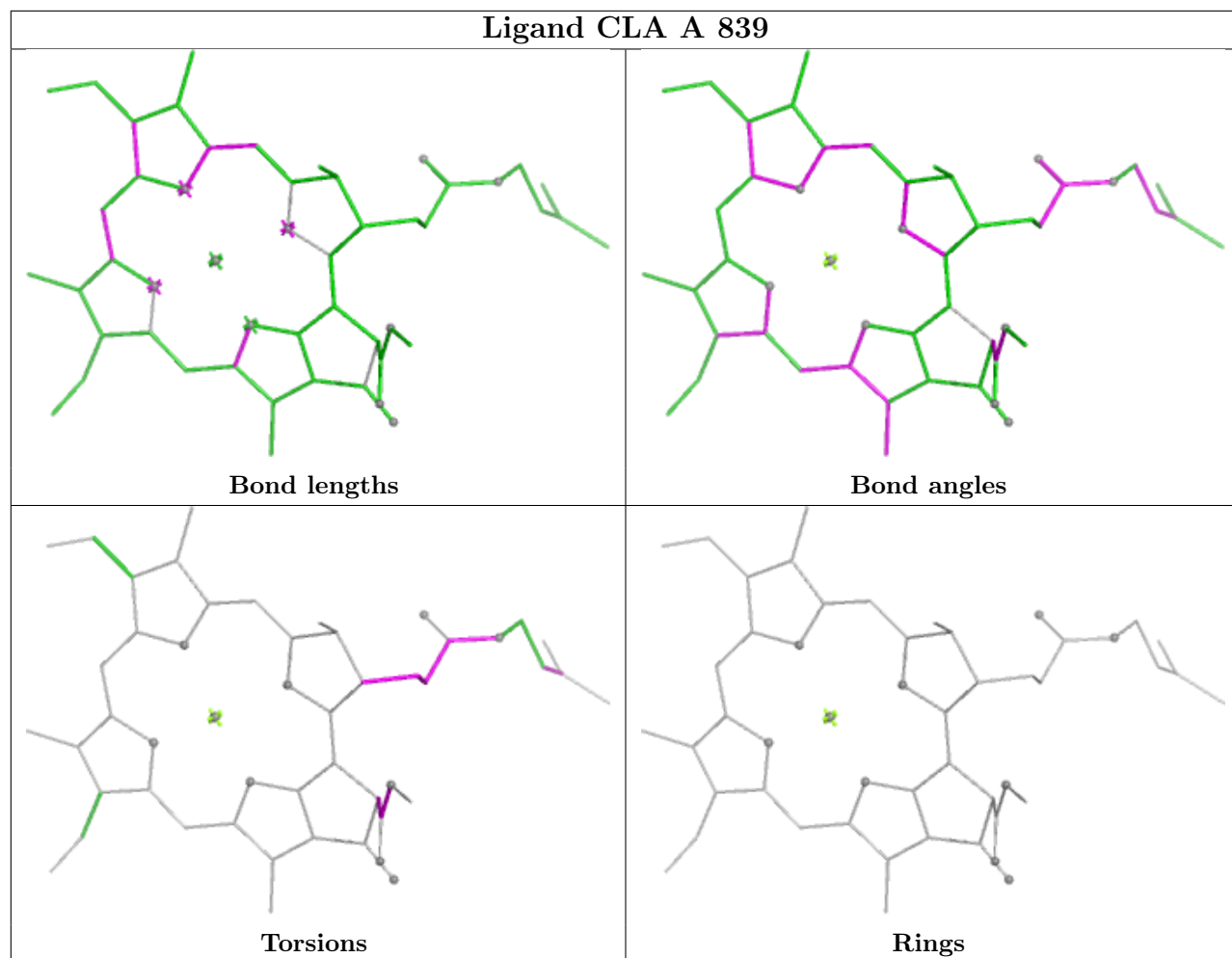
Bond angles



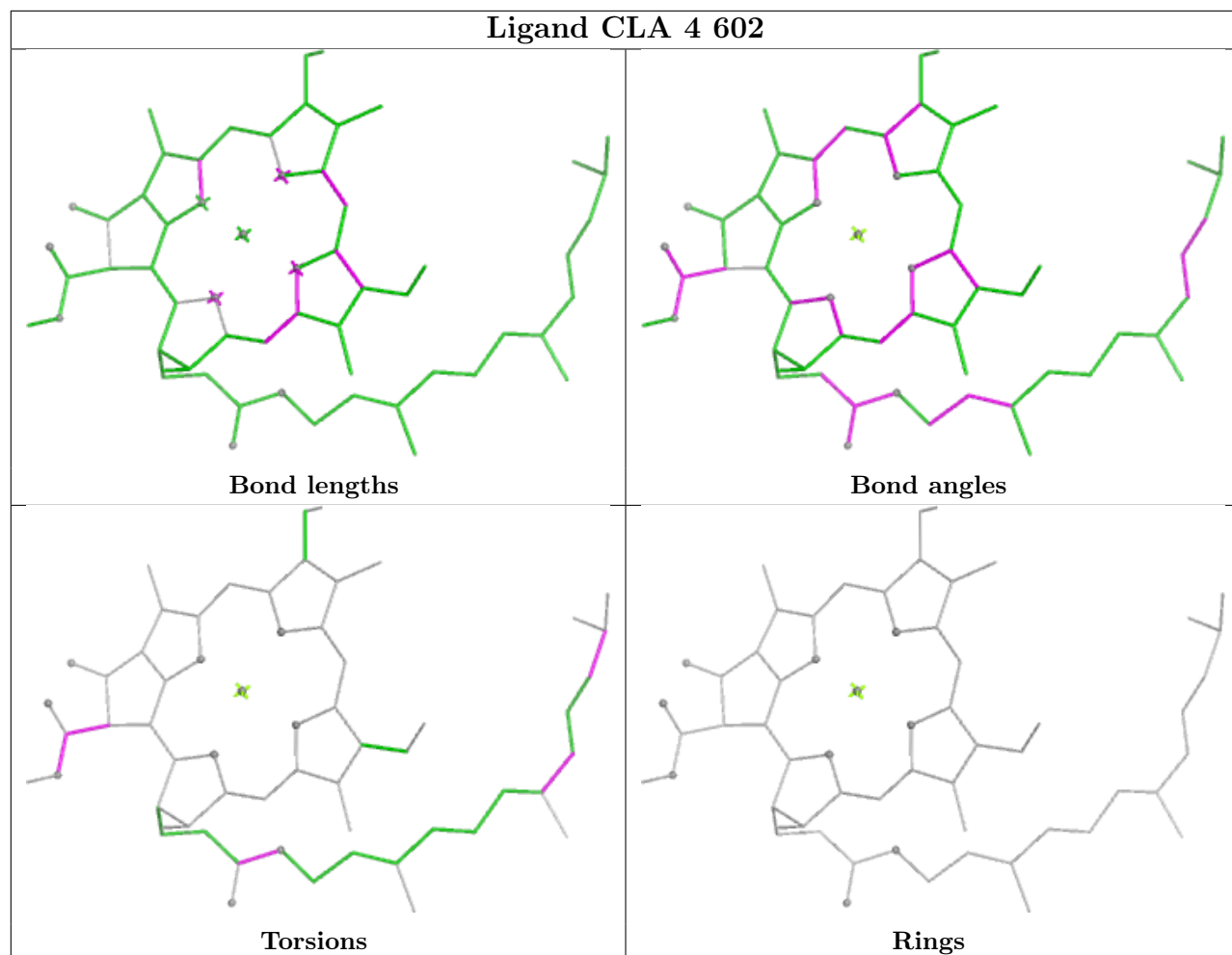
Torsions



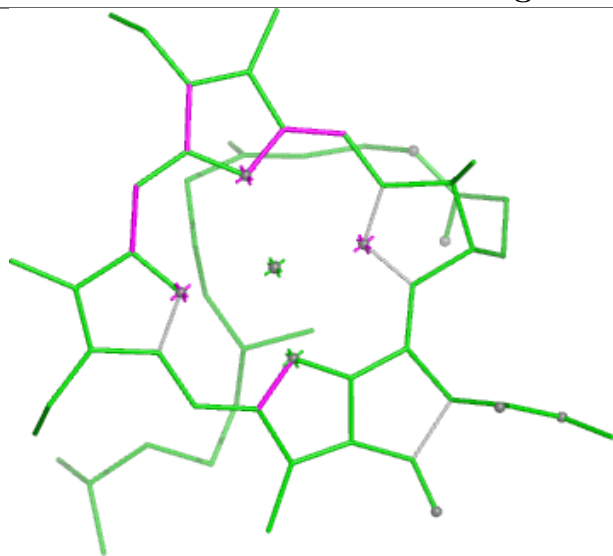
Rings



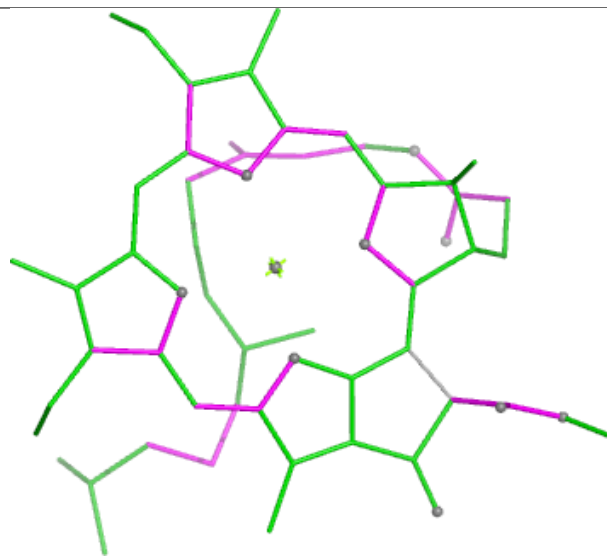
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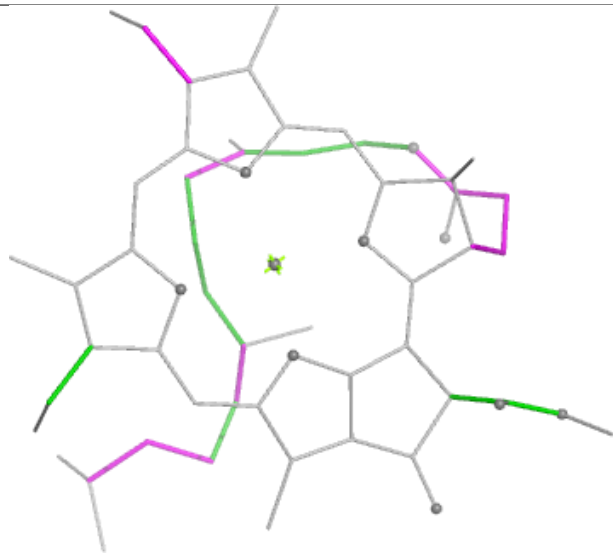
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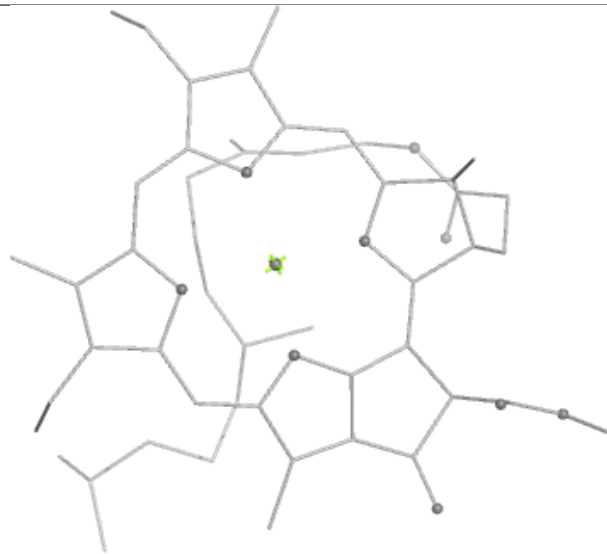
Bond lengths



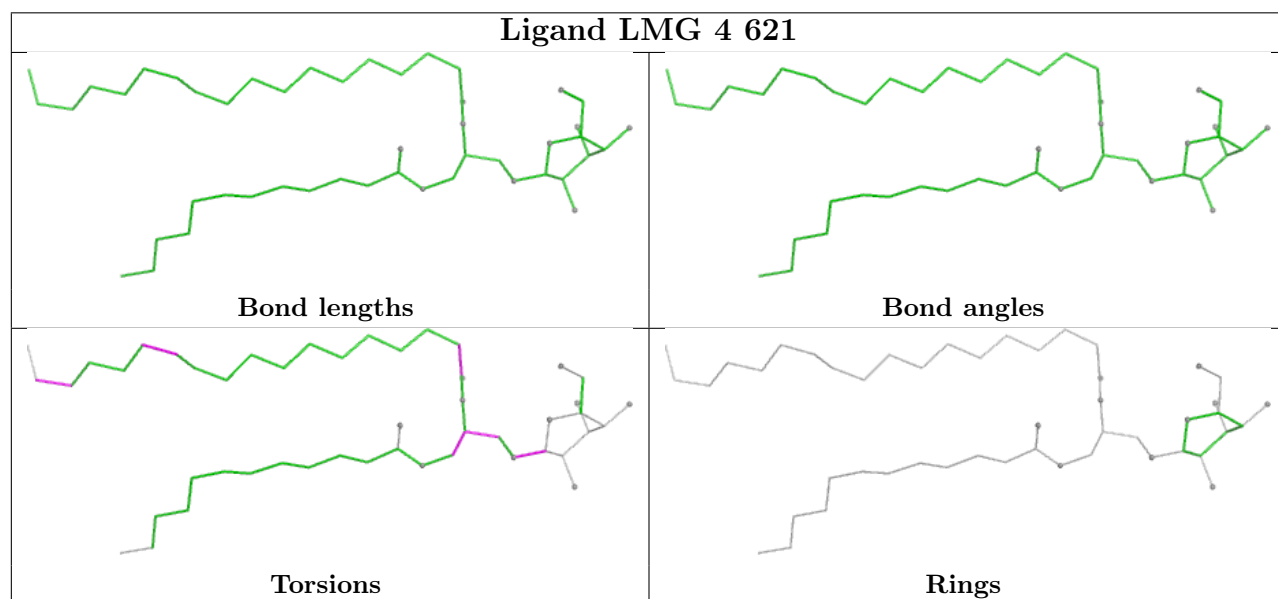
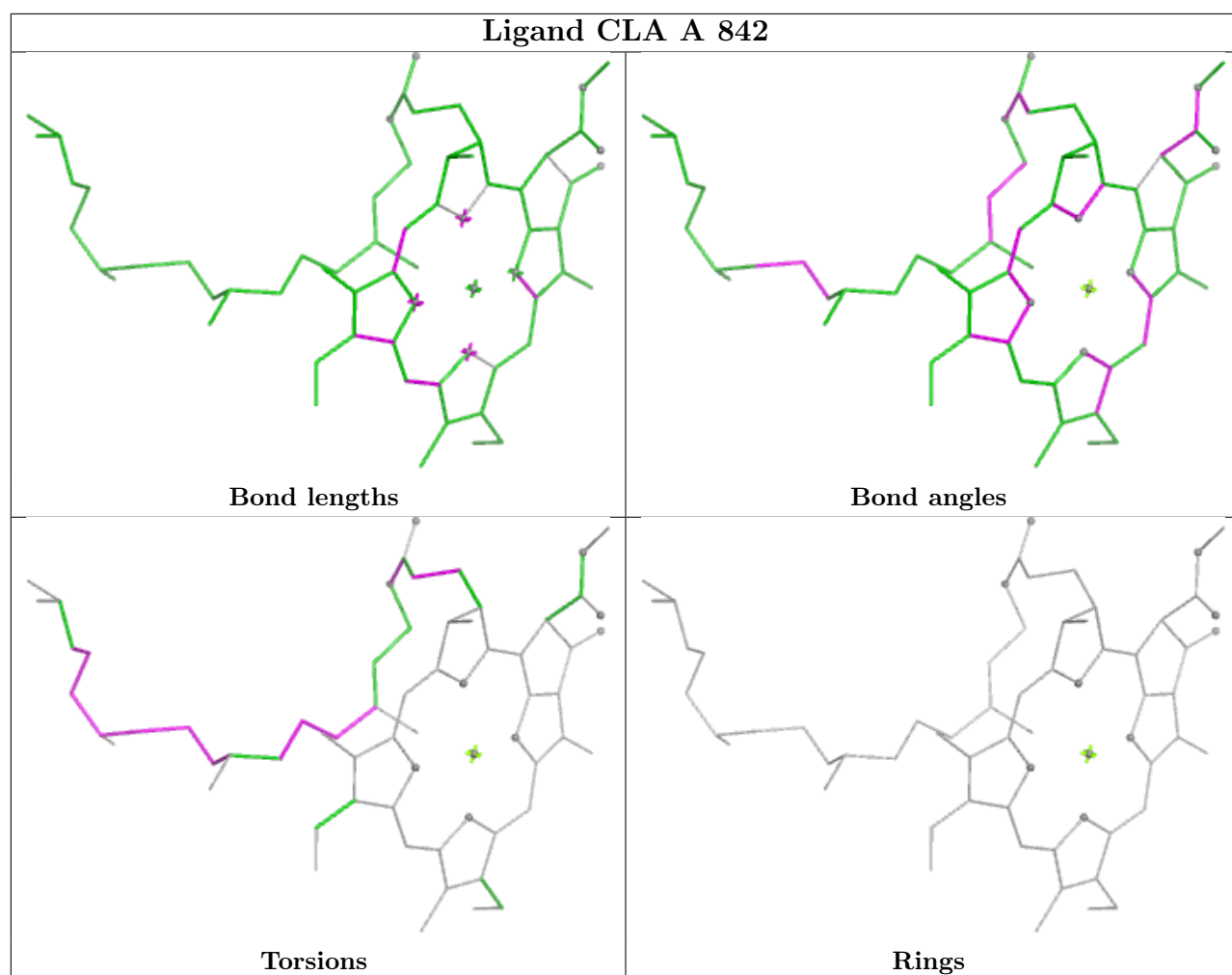
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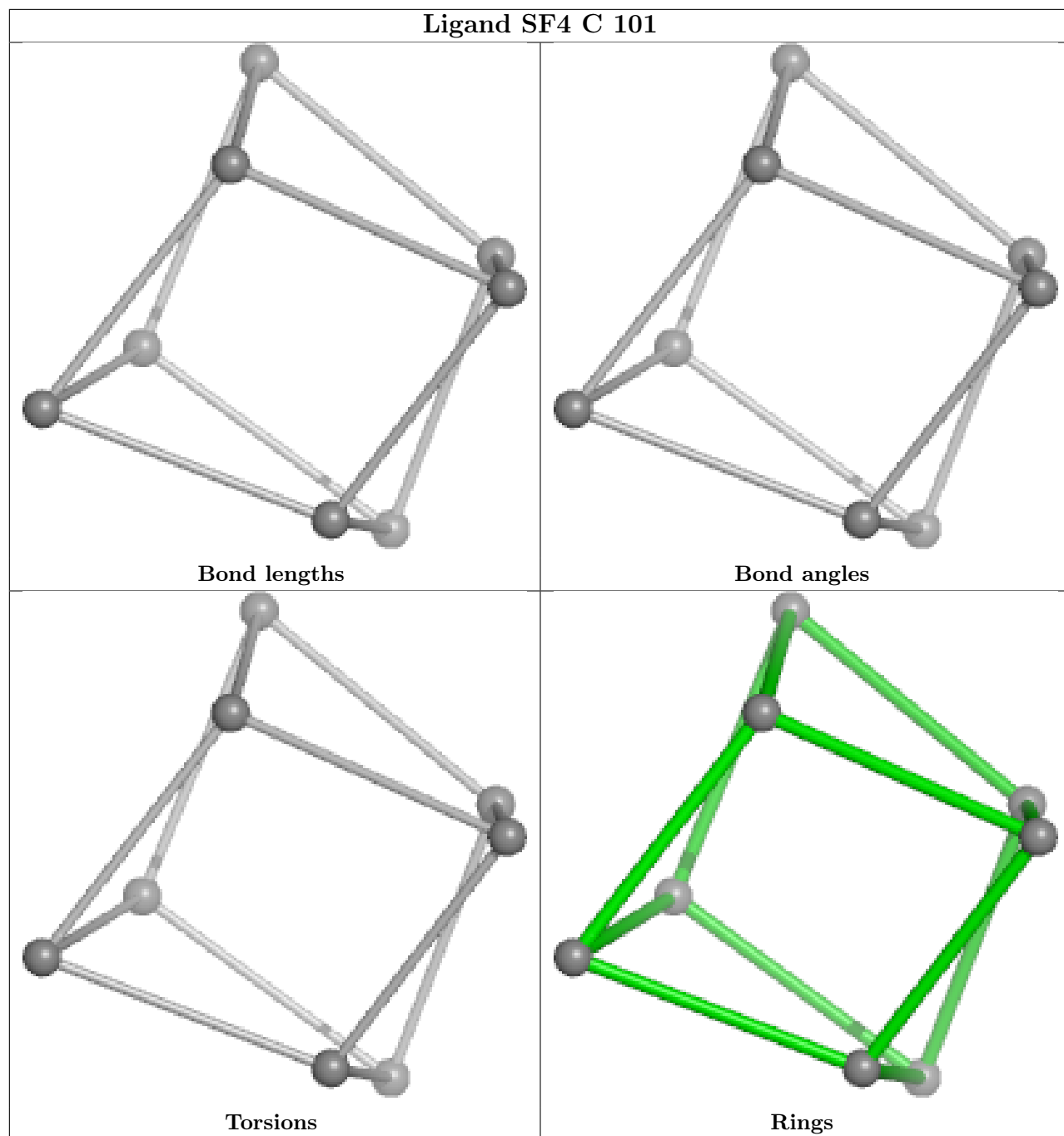


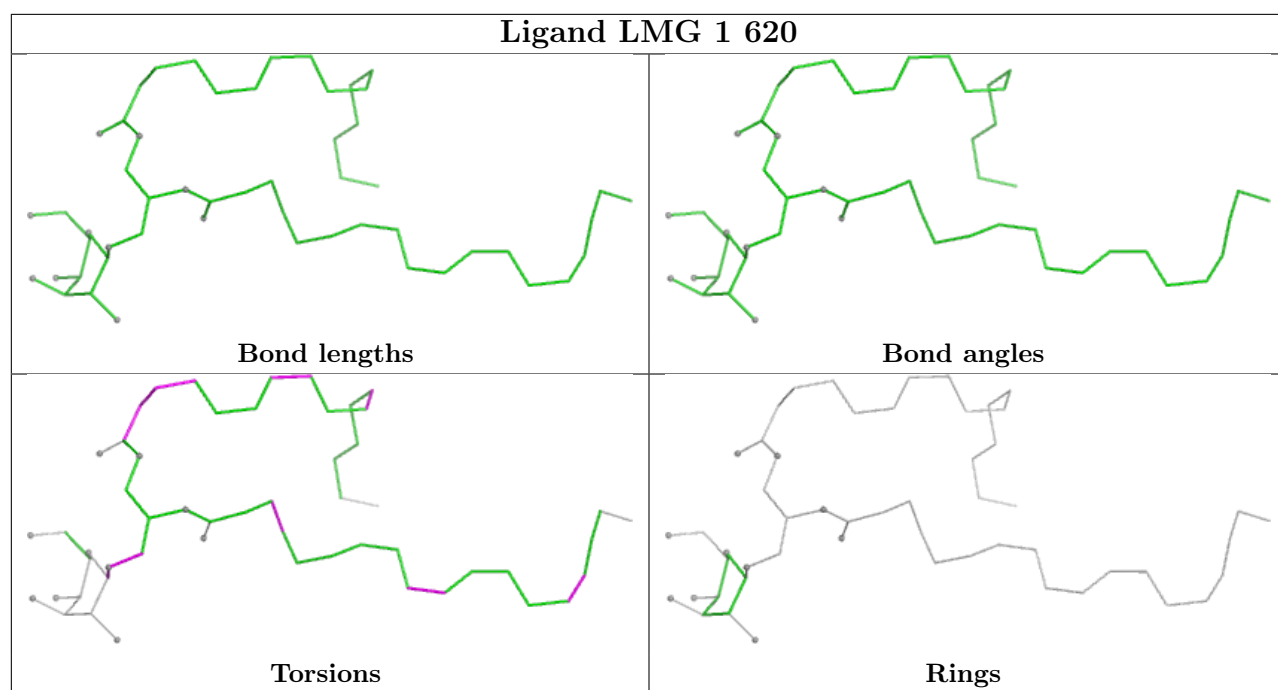
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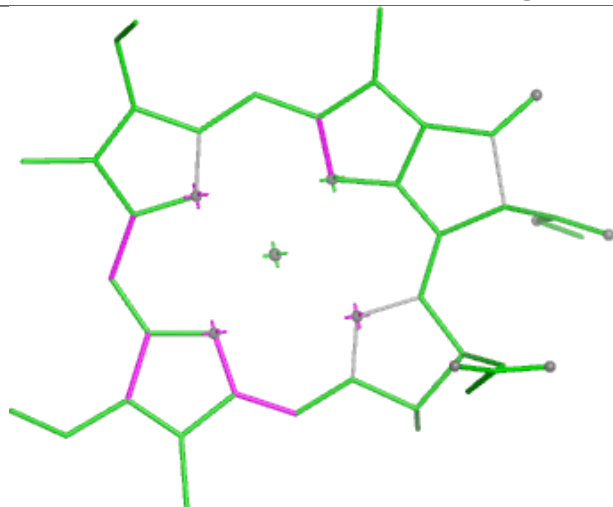
Rings



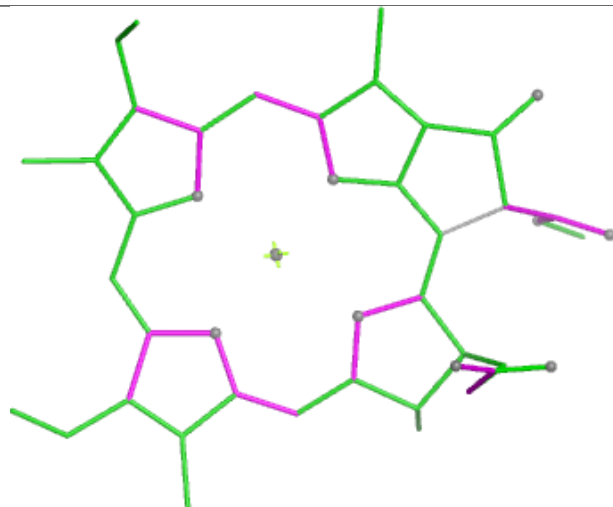




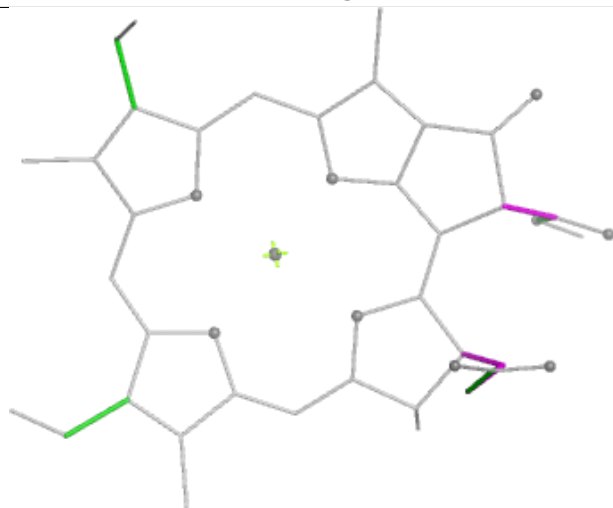
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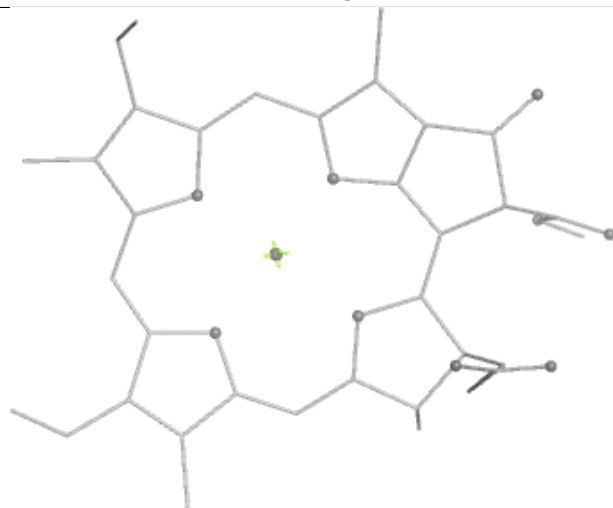
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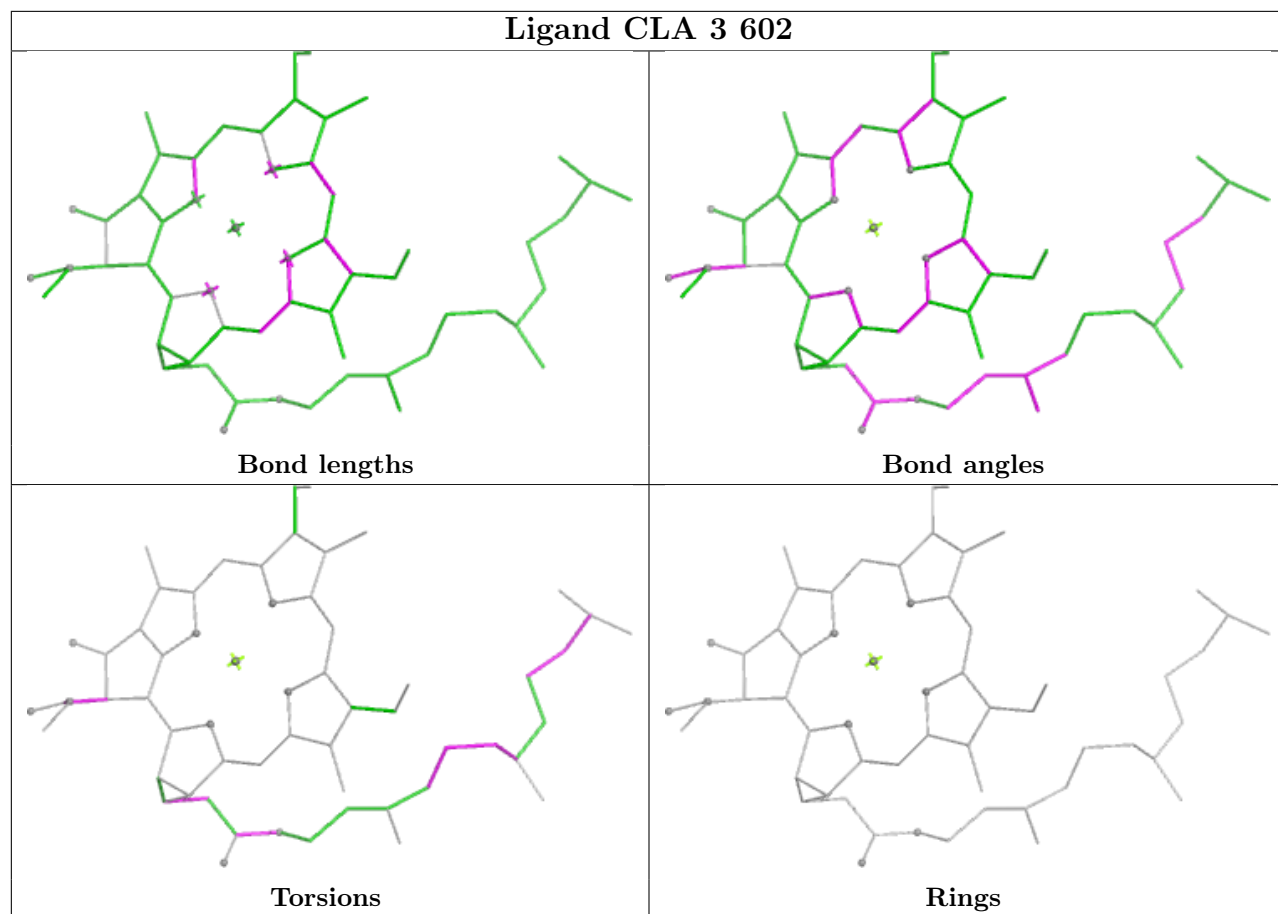
Bond angles



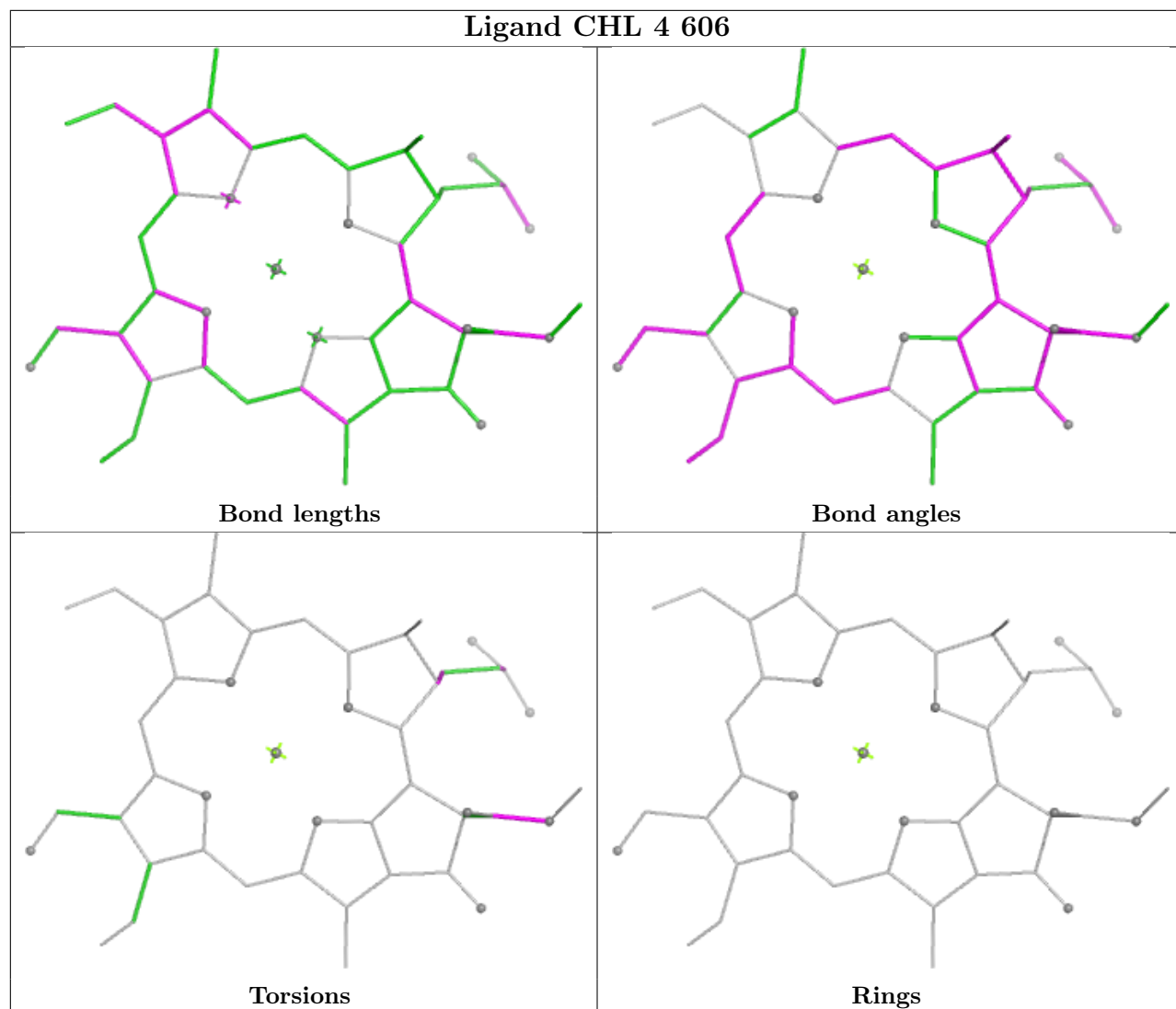
Torsions

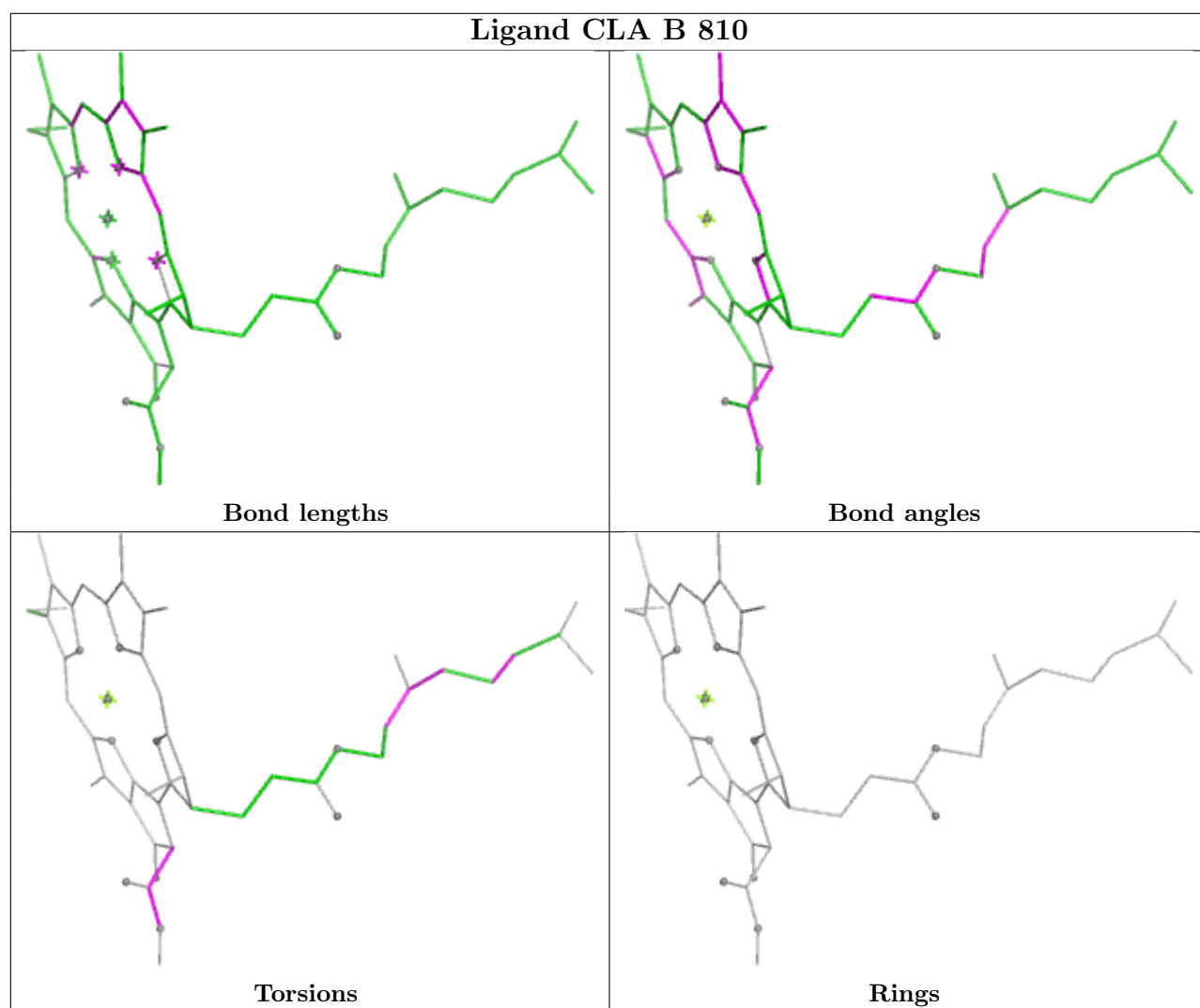


Rings

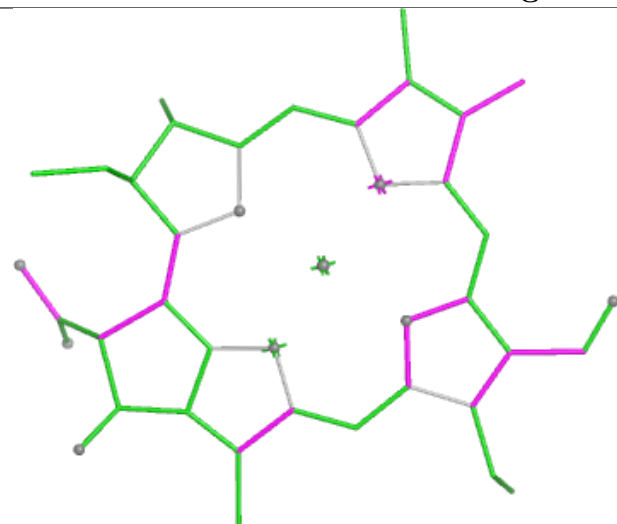


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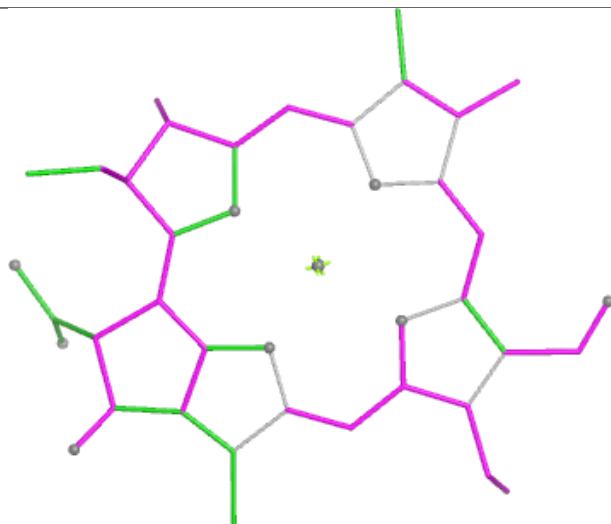




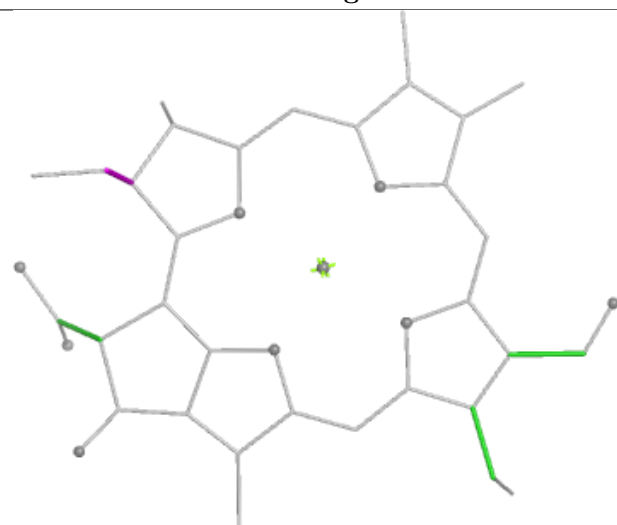
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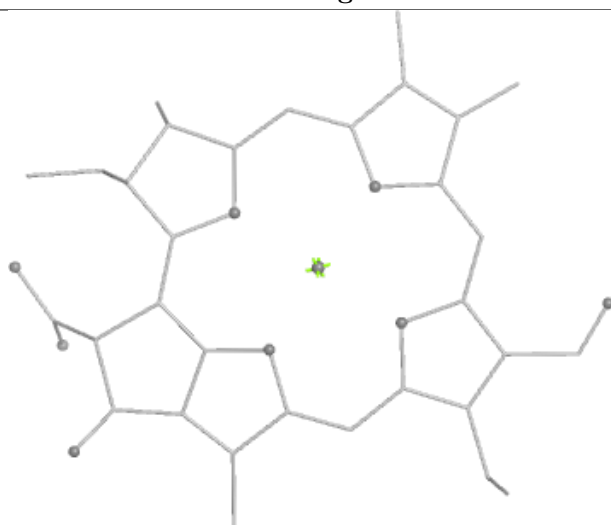
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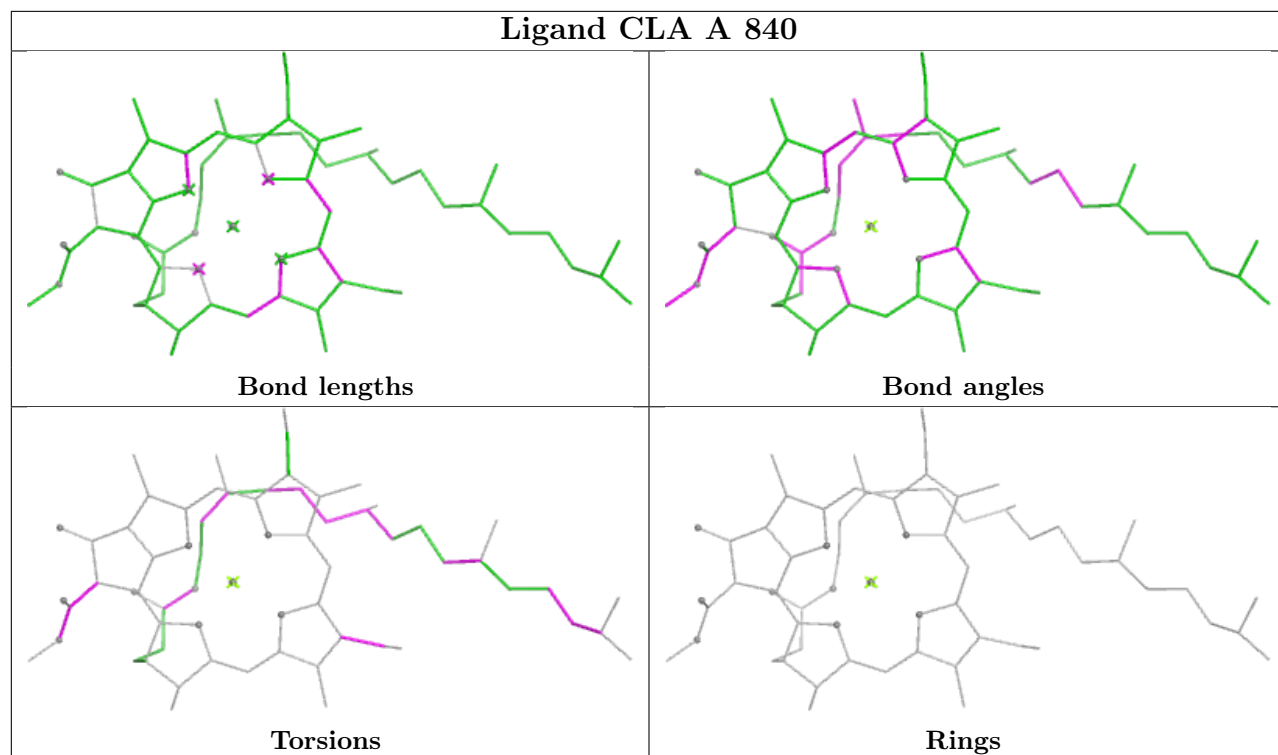
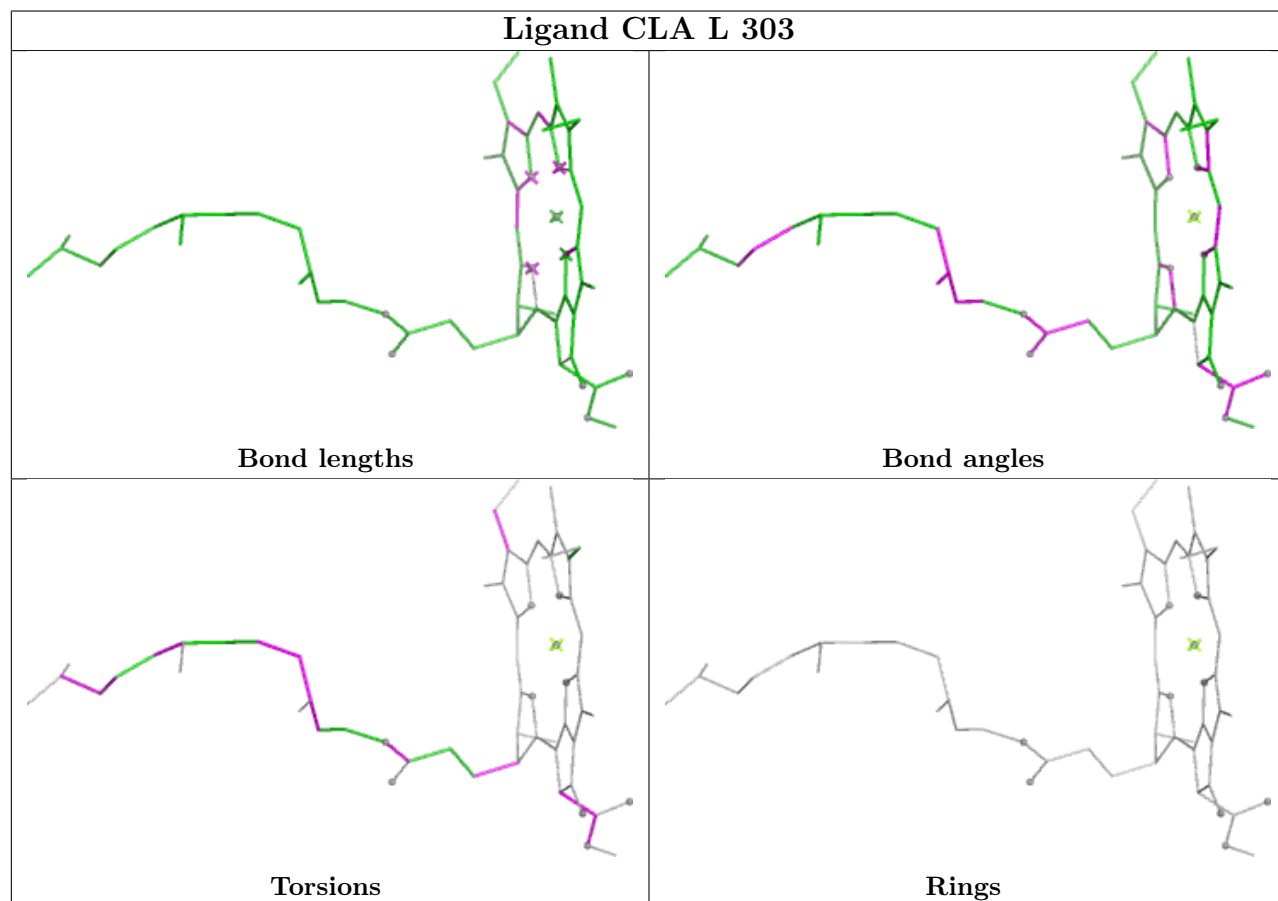
Bond angles



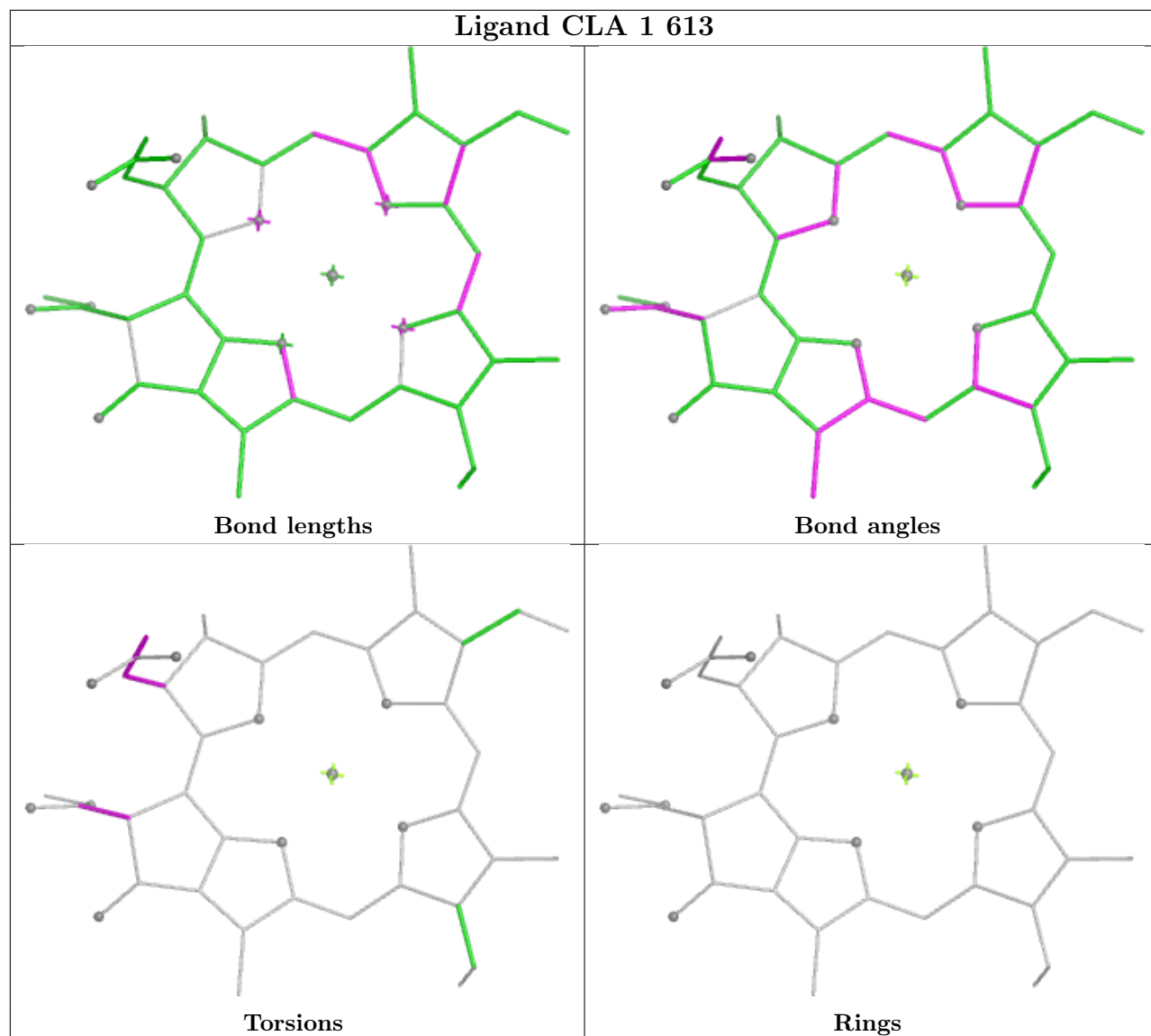
Torsions



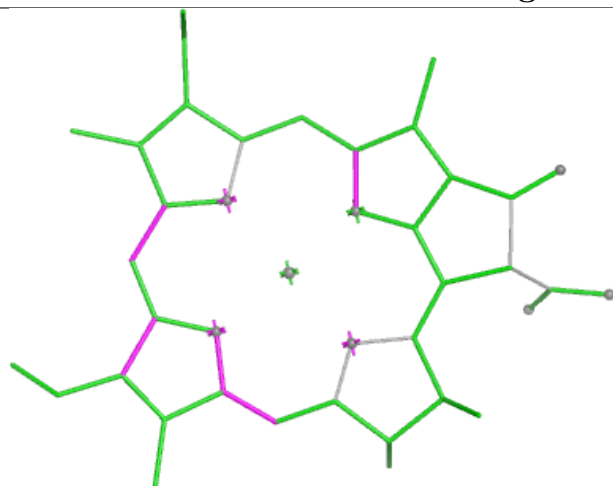
Rings

Ligand CLA A 840**Ligand CLA L 303**

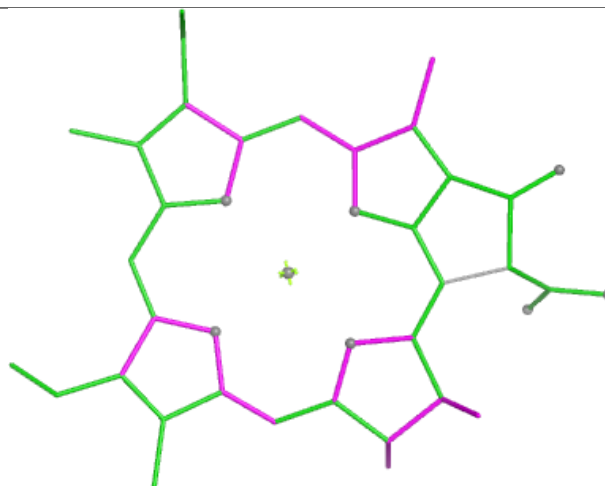
Ligand CLA 1 613



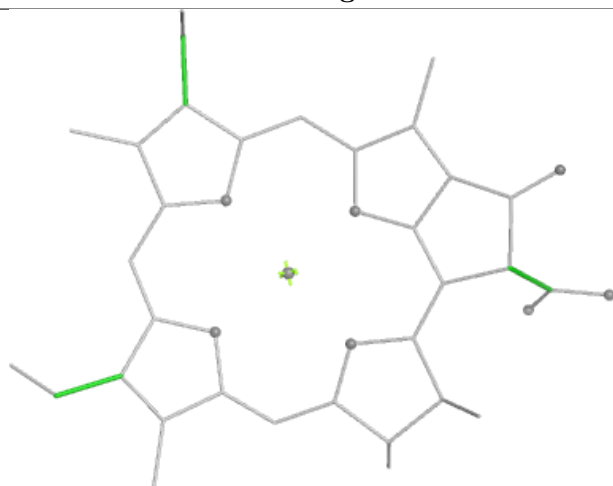
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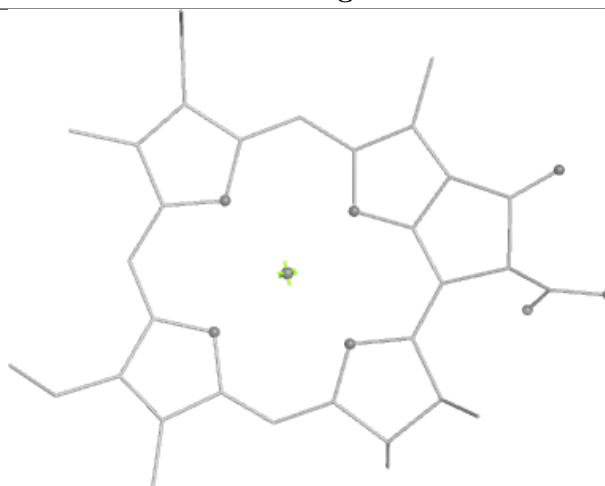
Bond lengths



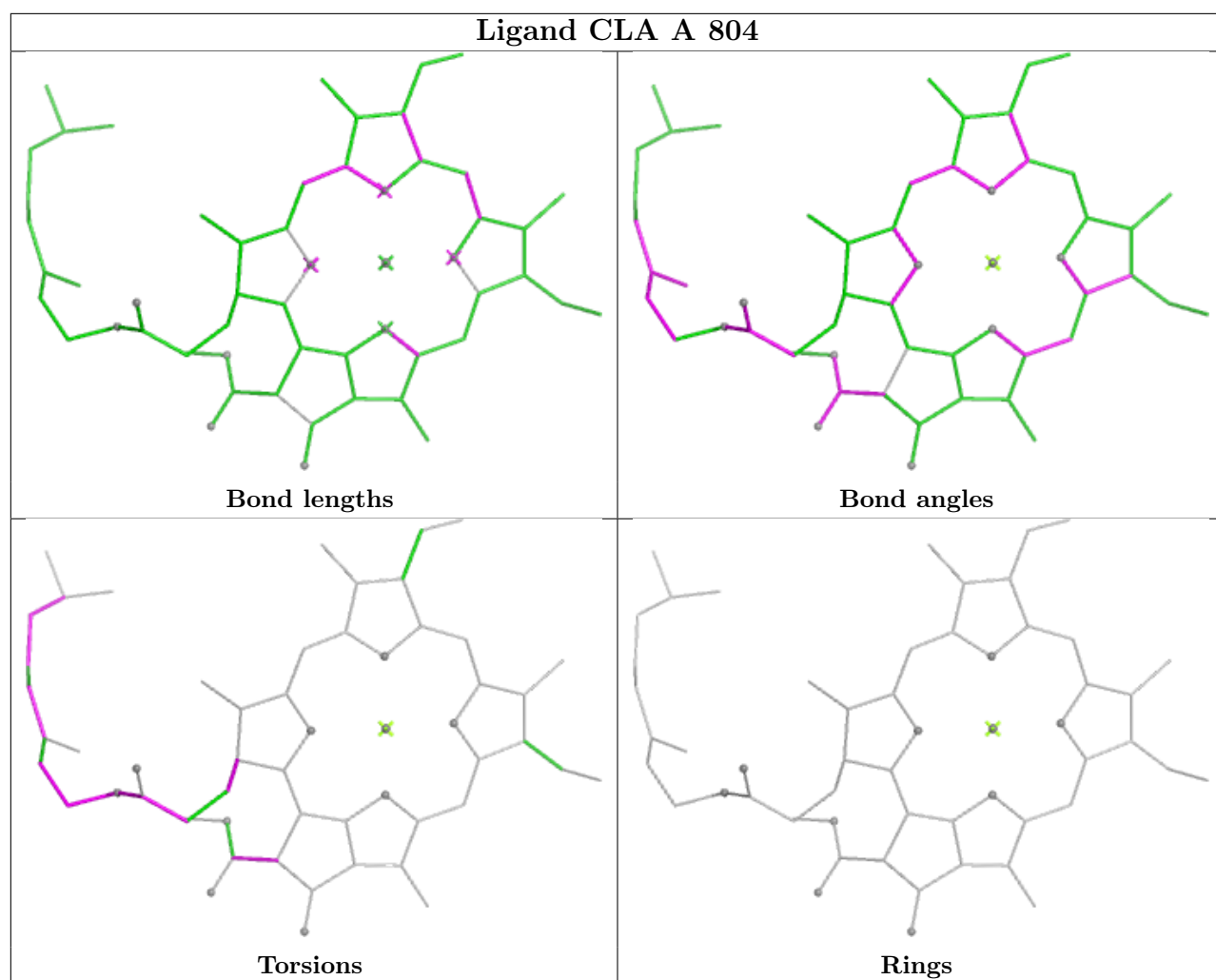
Bond angles

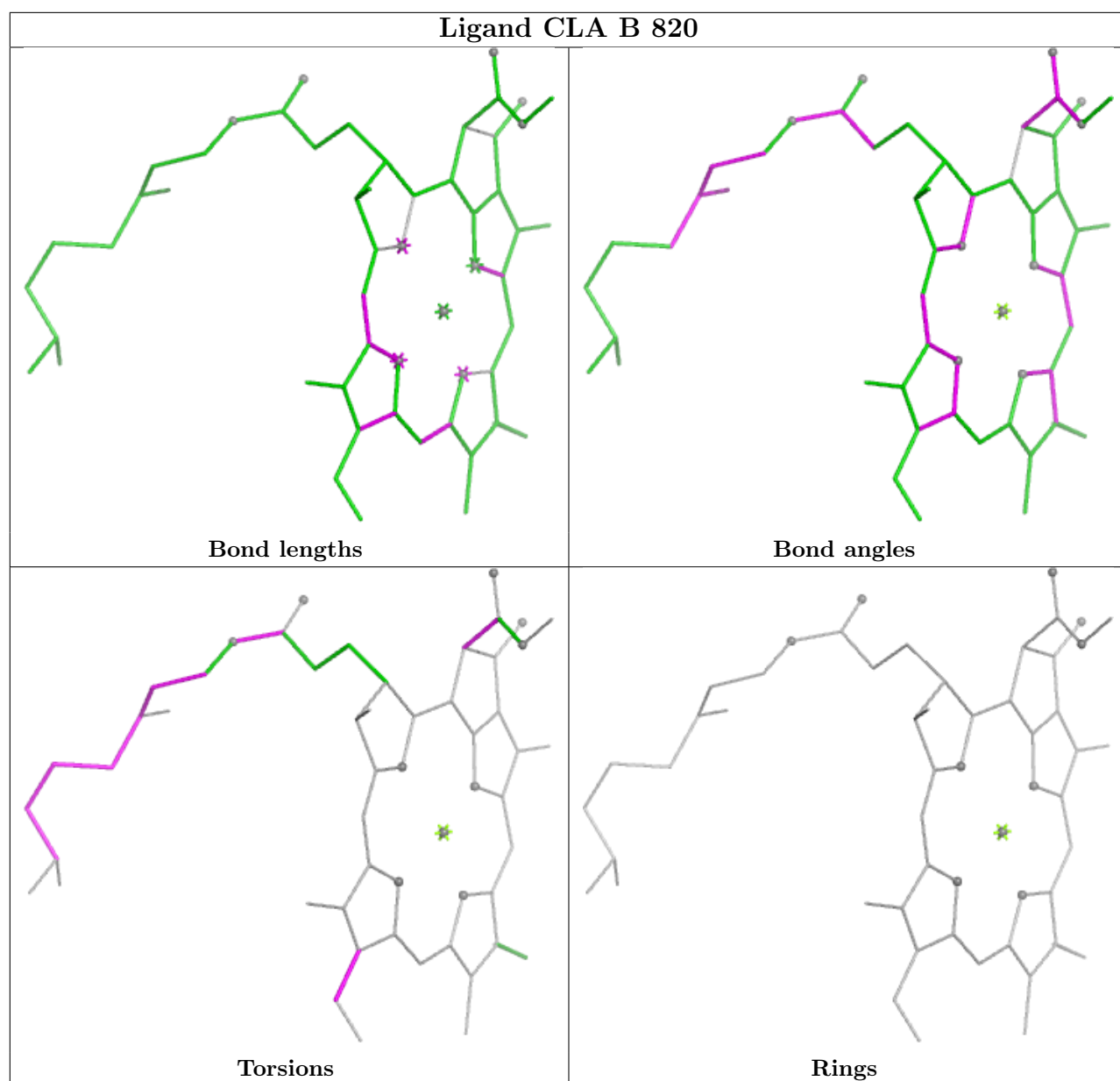


Torsions

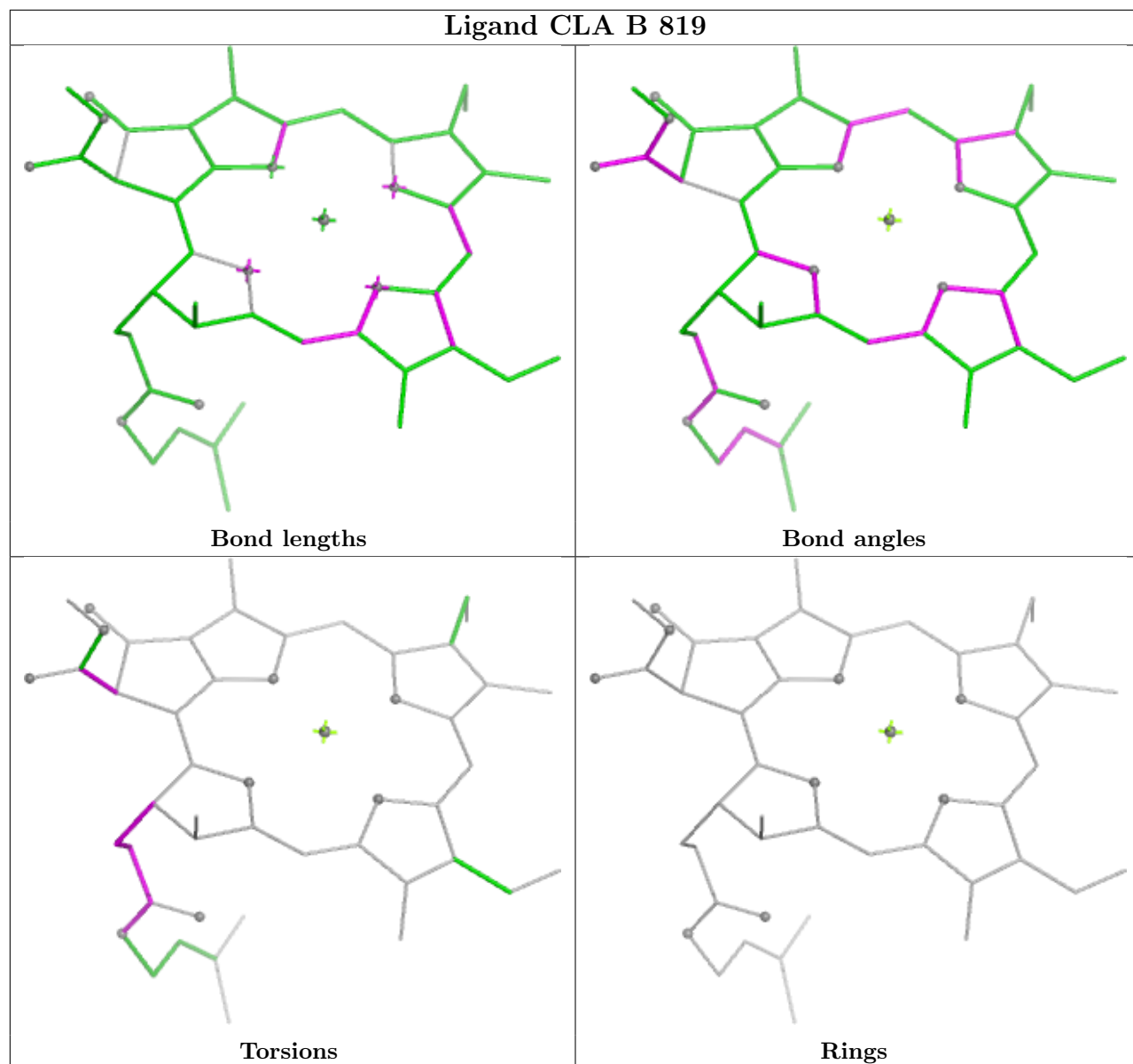


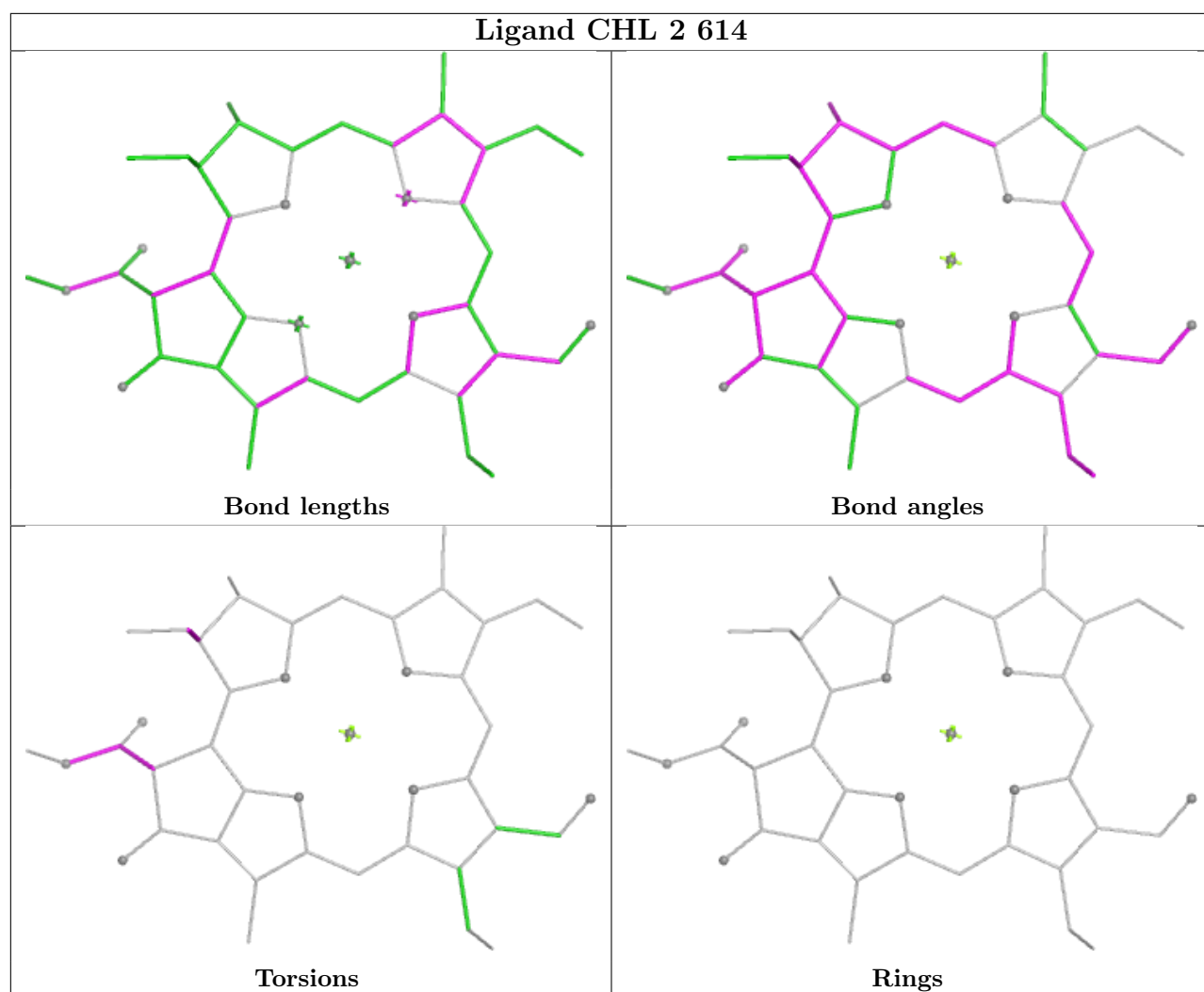
Rings



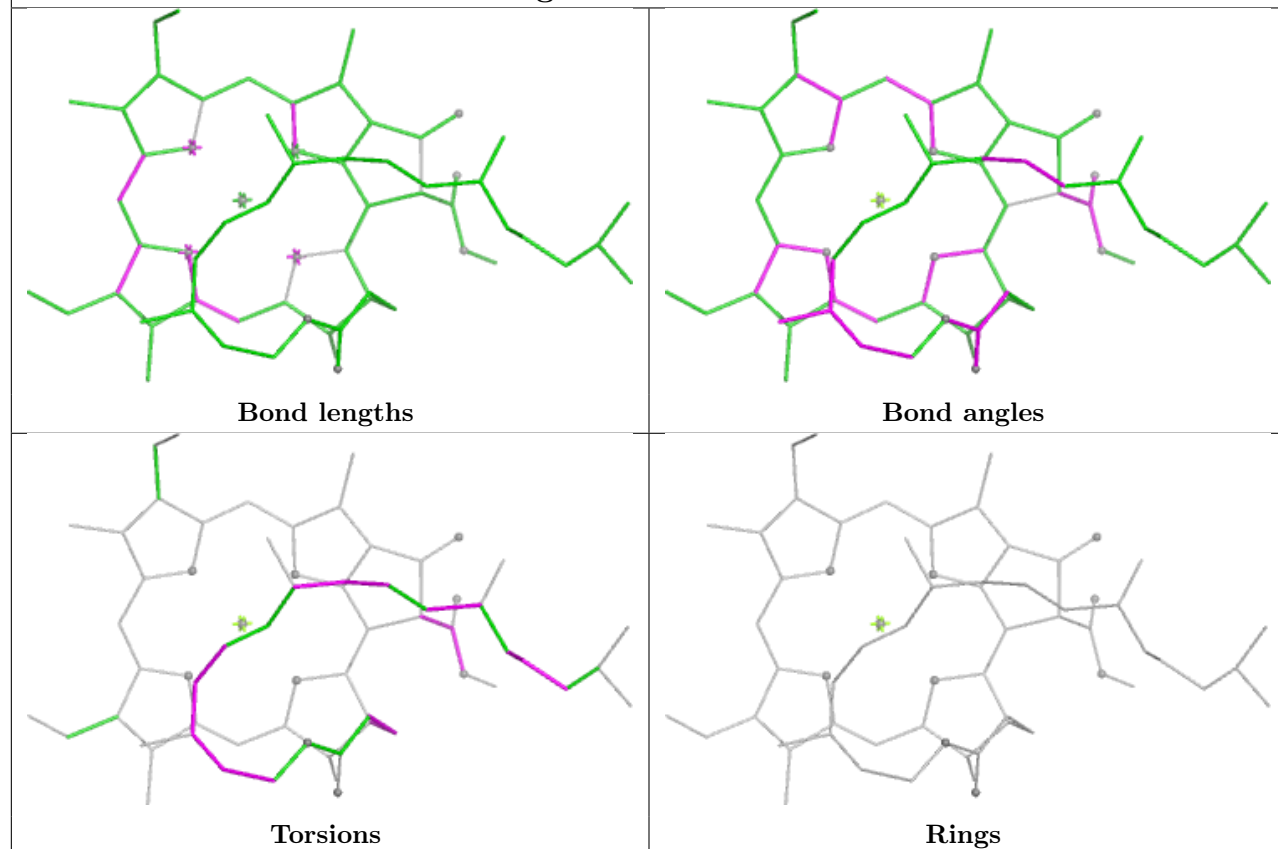


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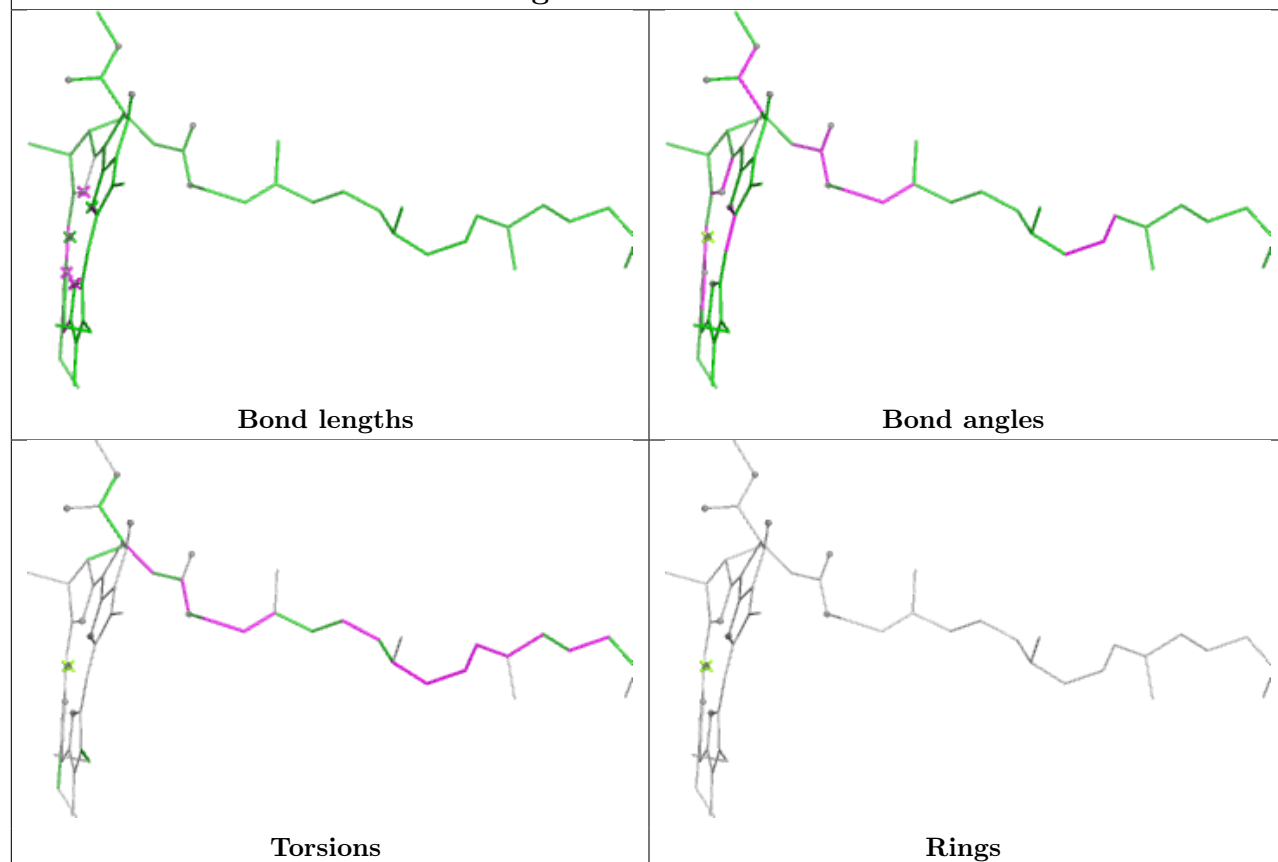




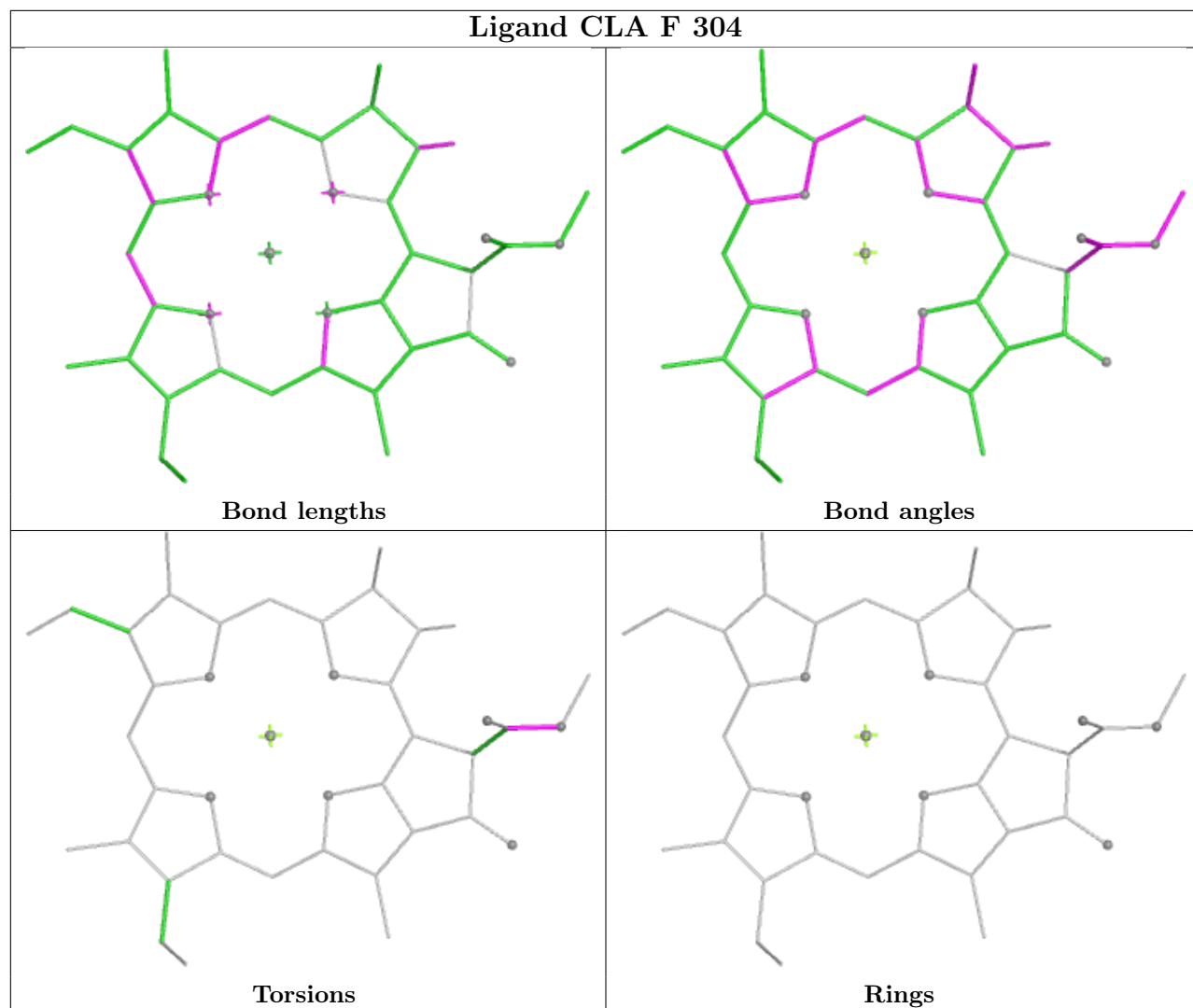
Ligand CLA 2 604



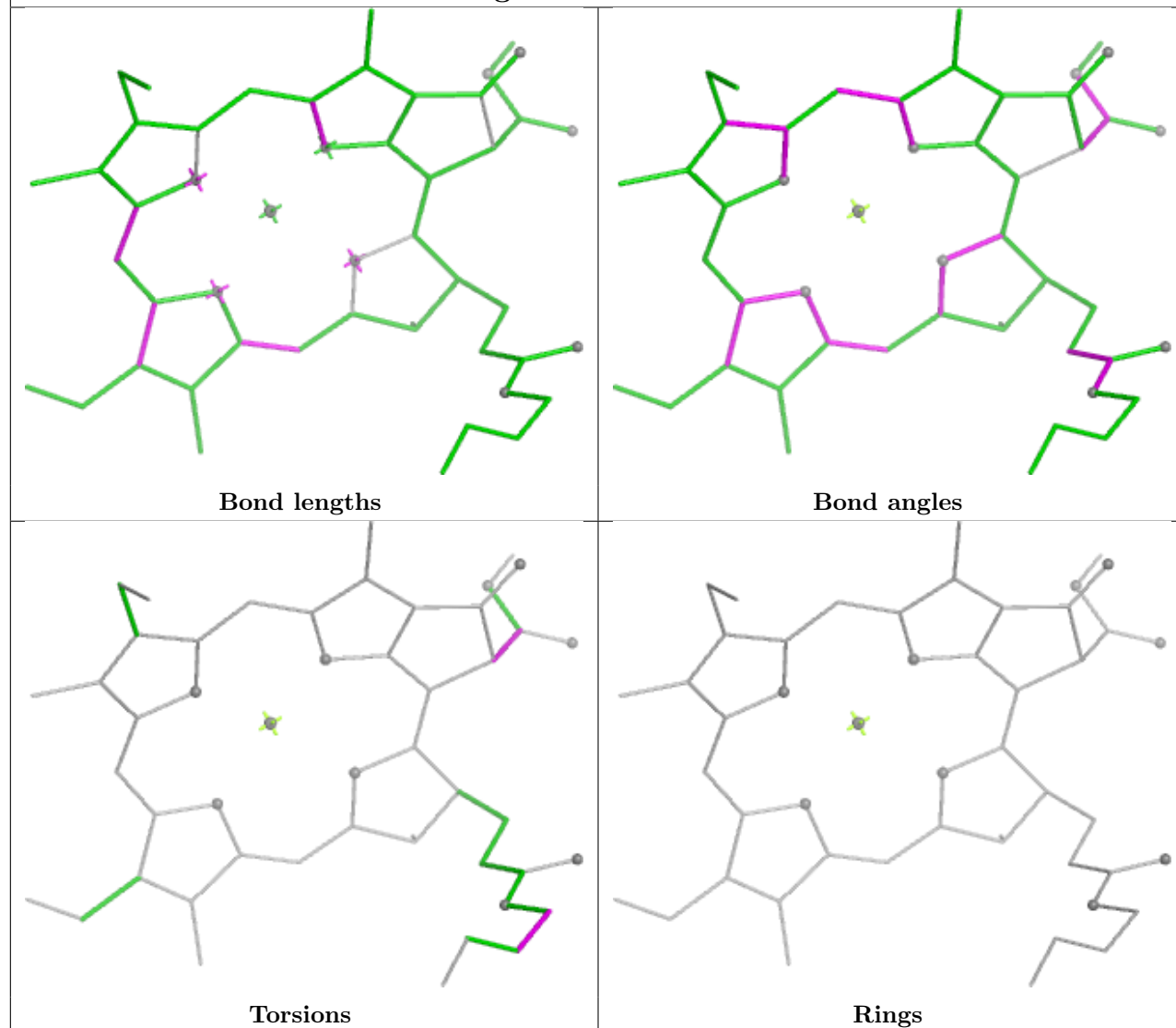
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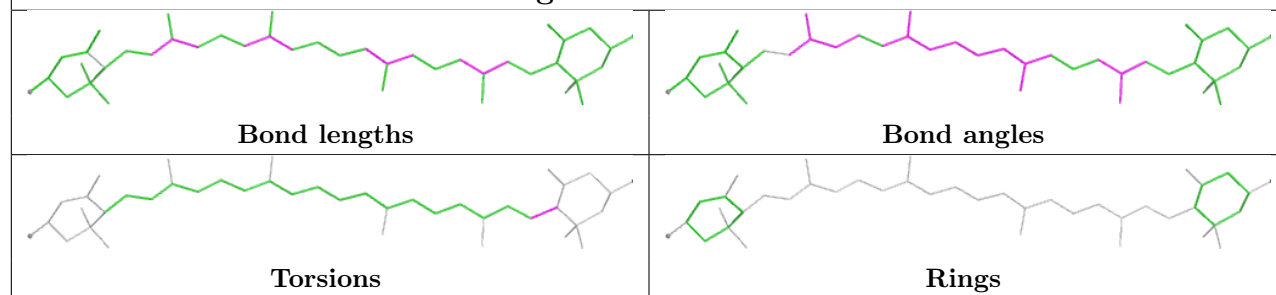
Ligand CLA F 304

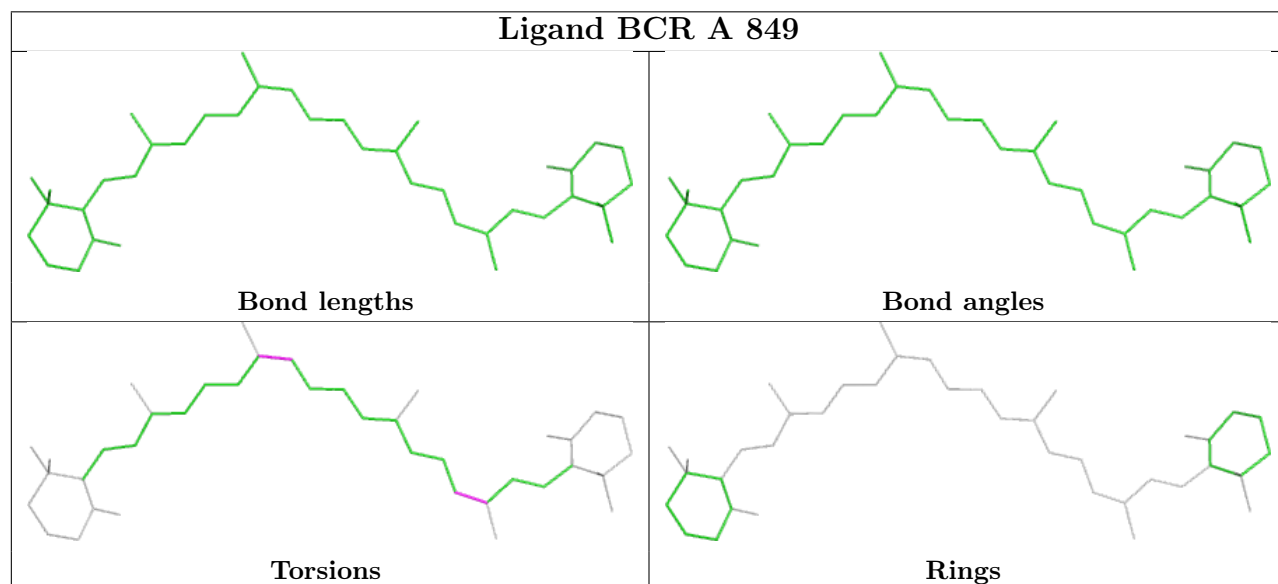
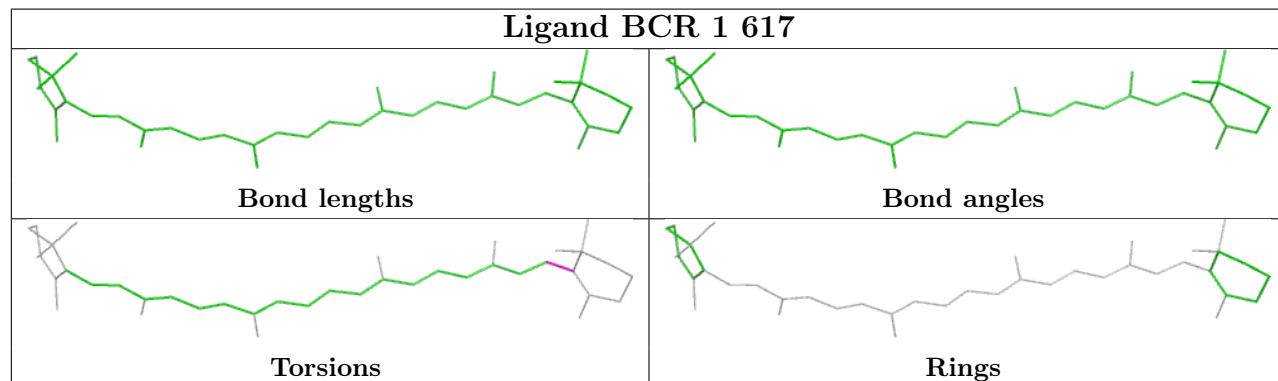
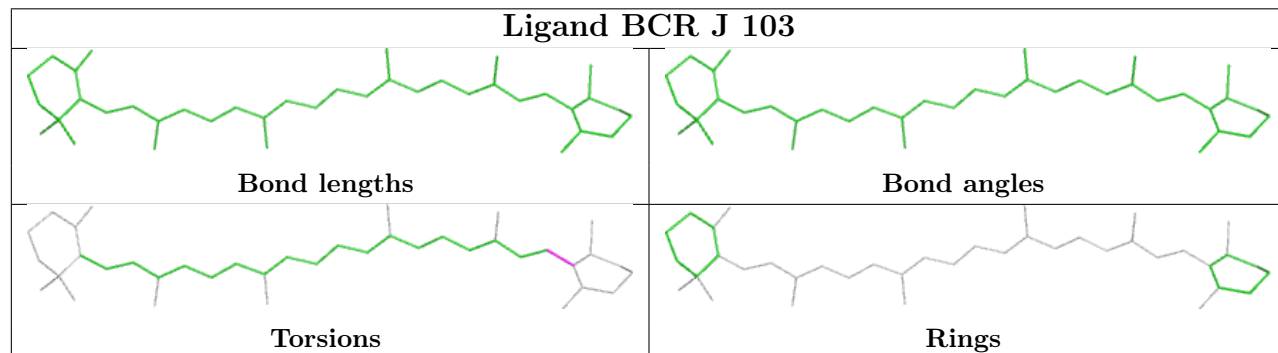
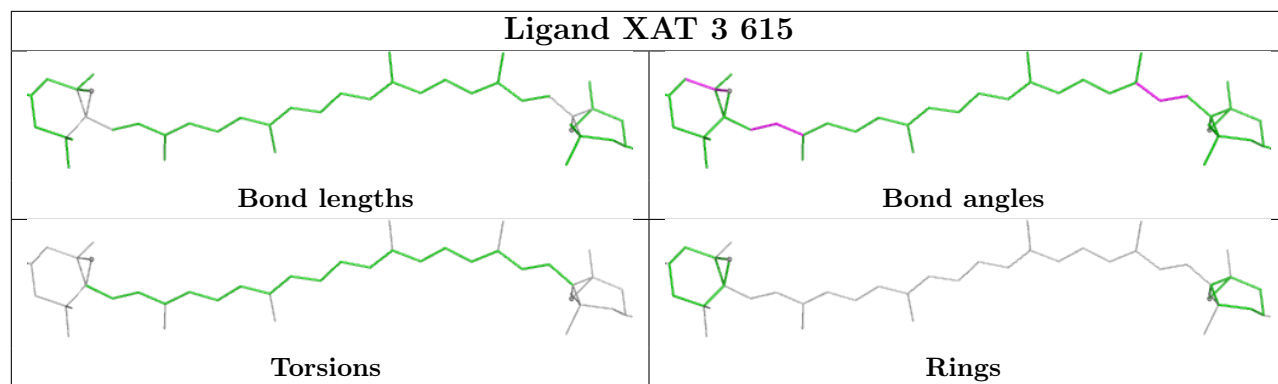


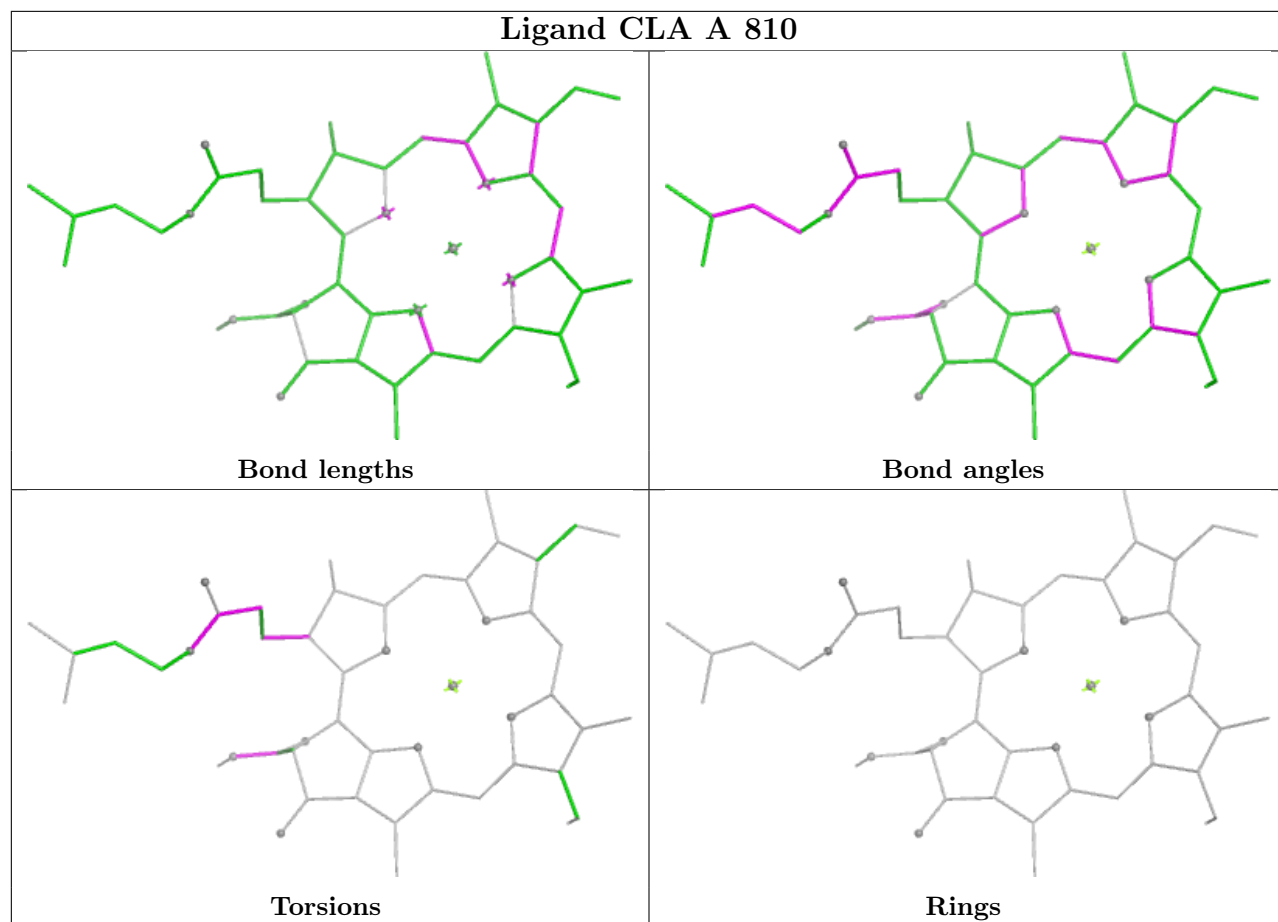
Ligand CLA 1 604



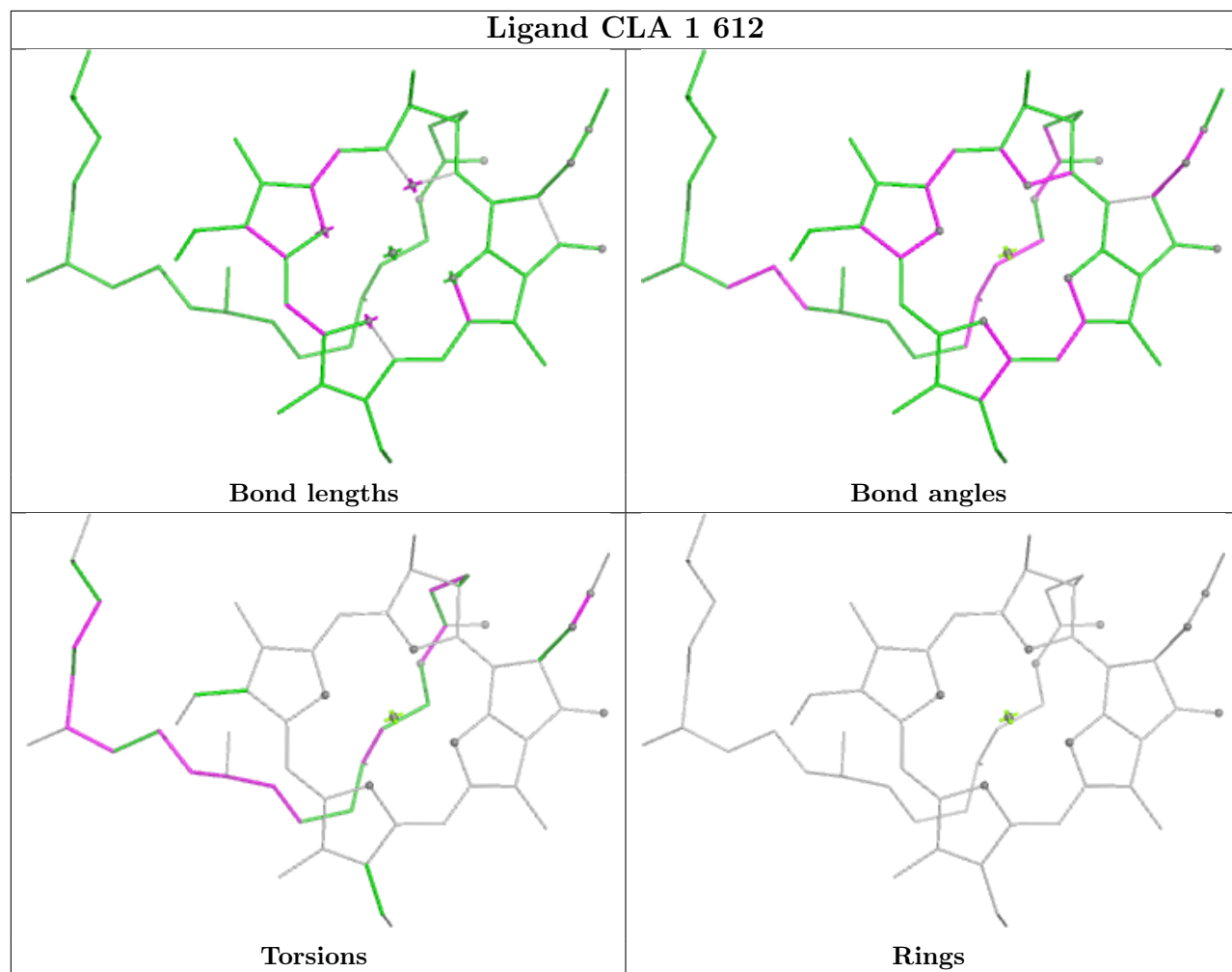
Ligand LUT 1 619



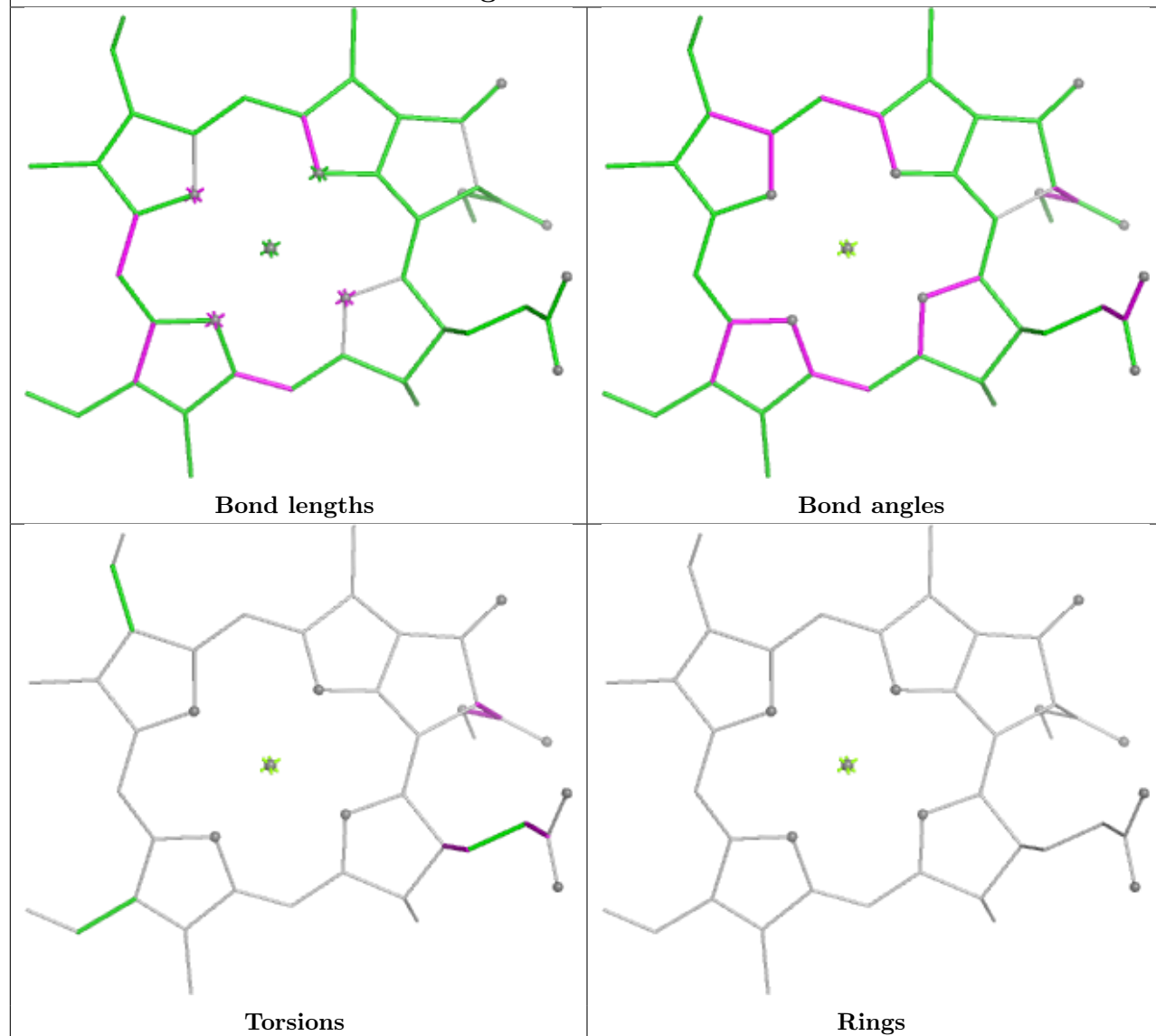




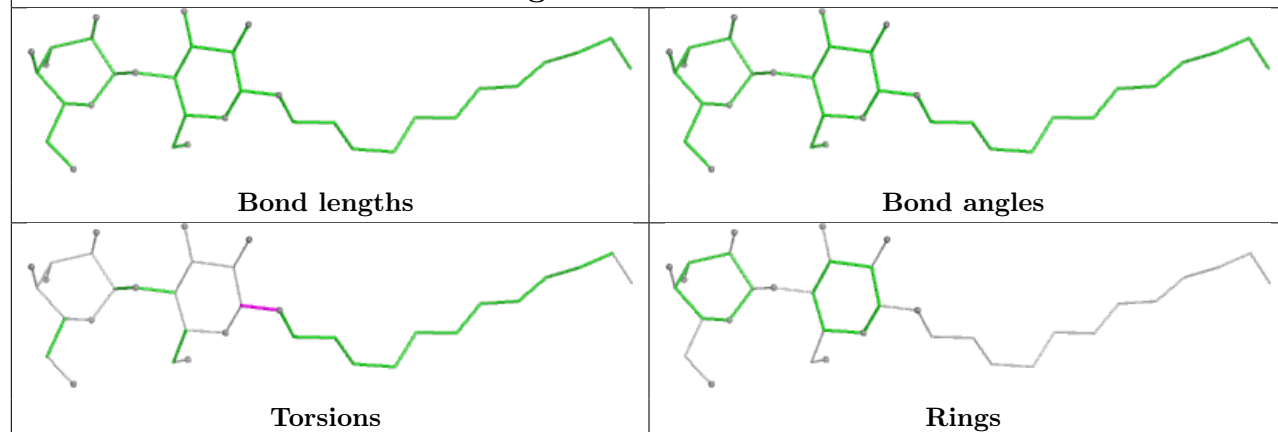
Ligand CLA 1 612

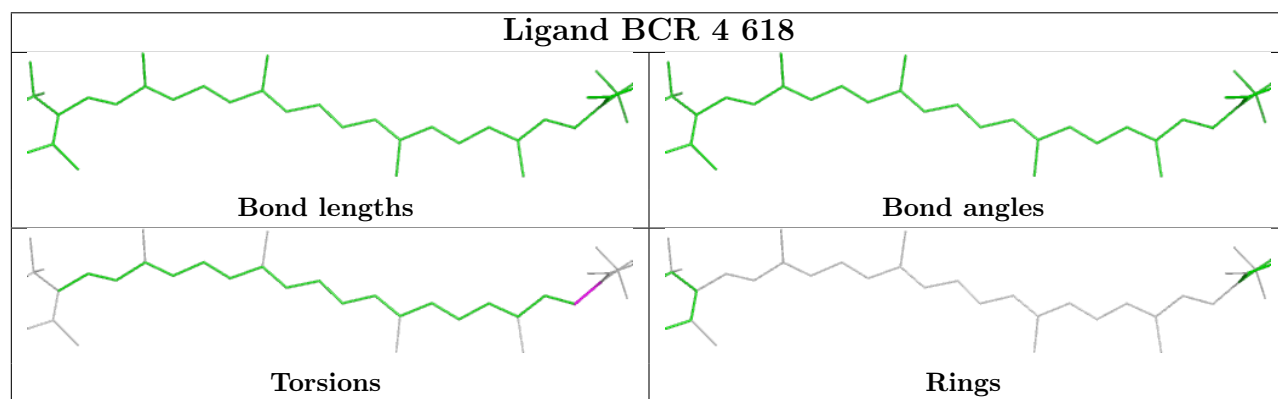
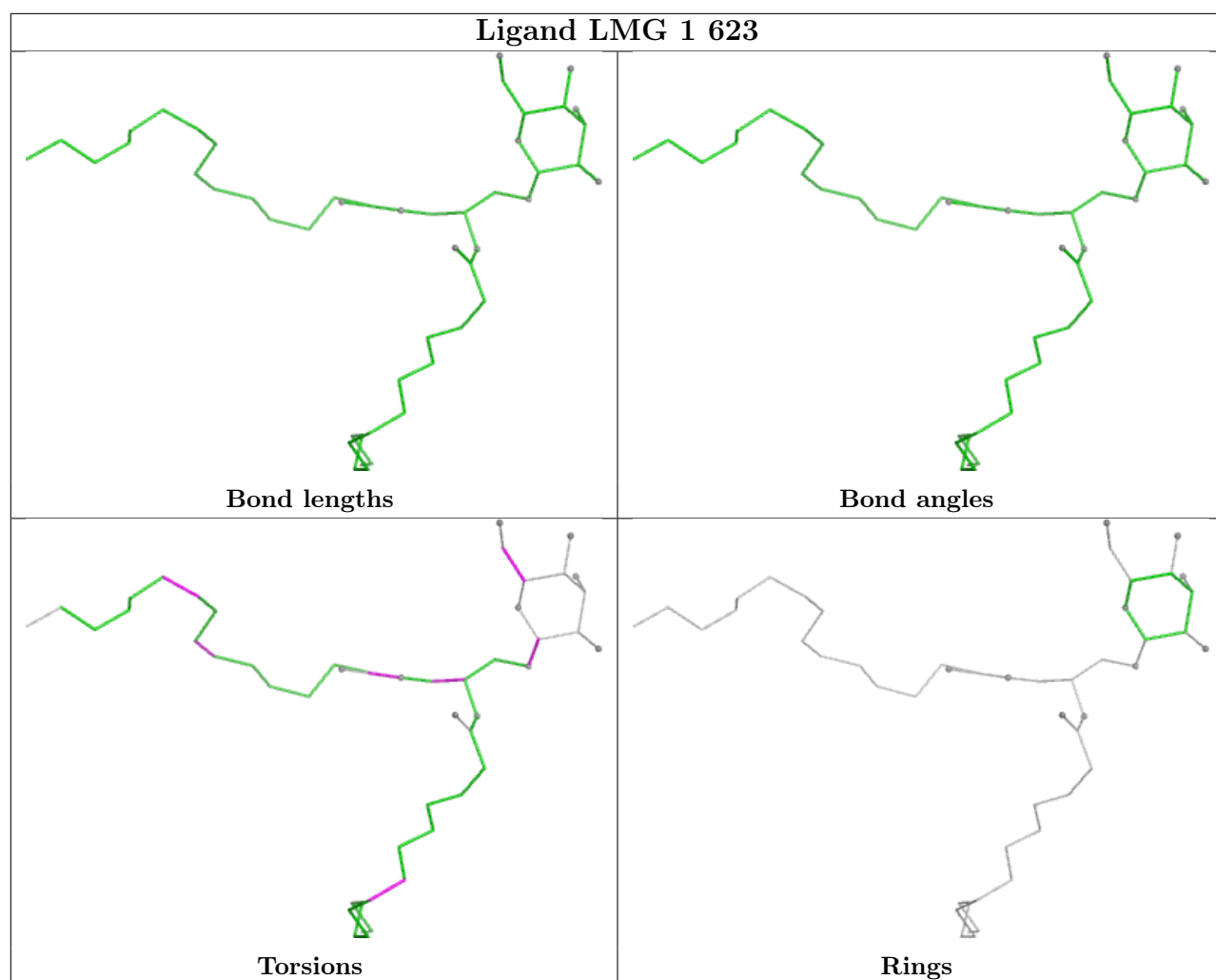


Ligand CLA K 202

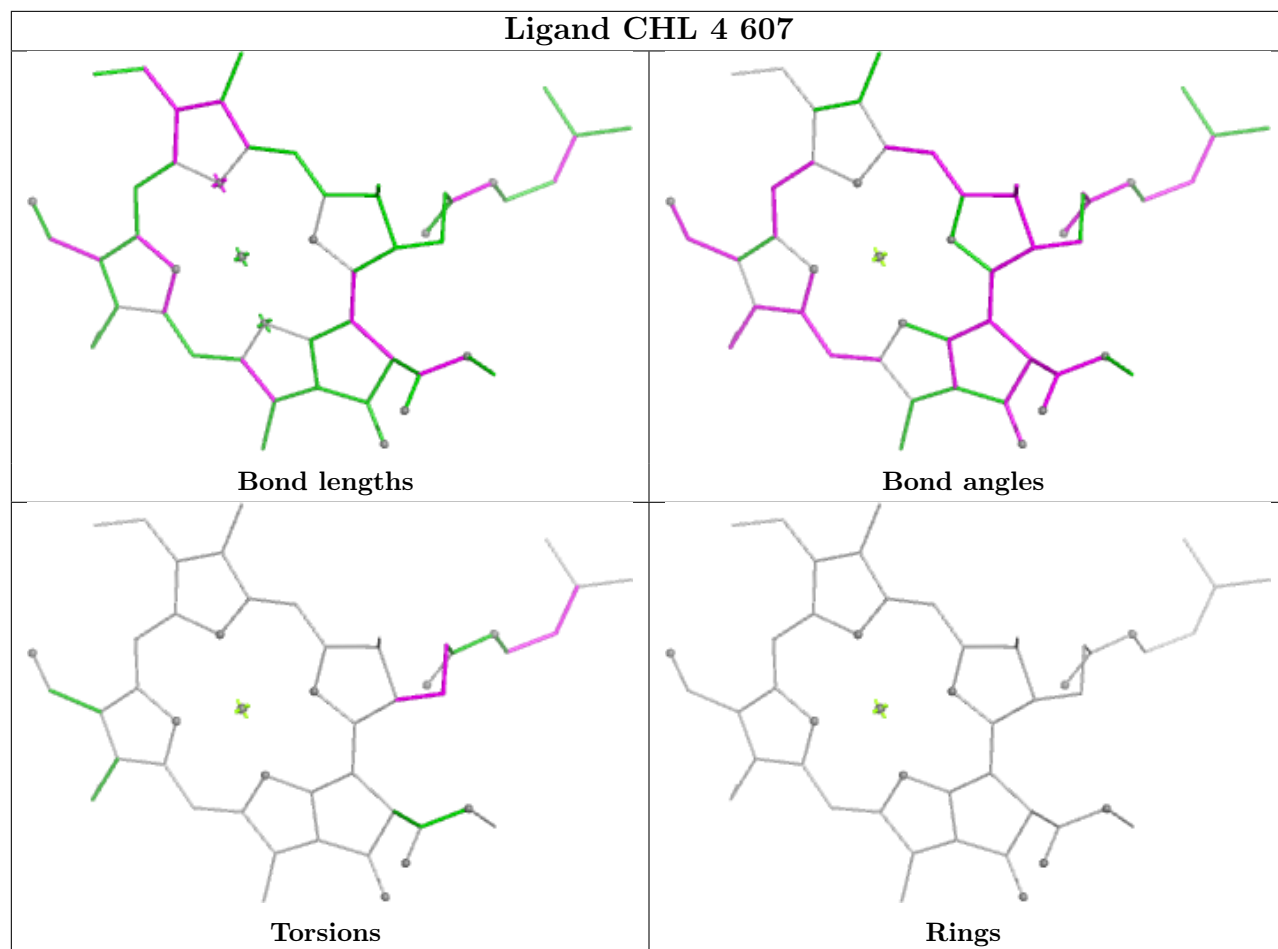


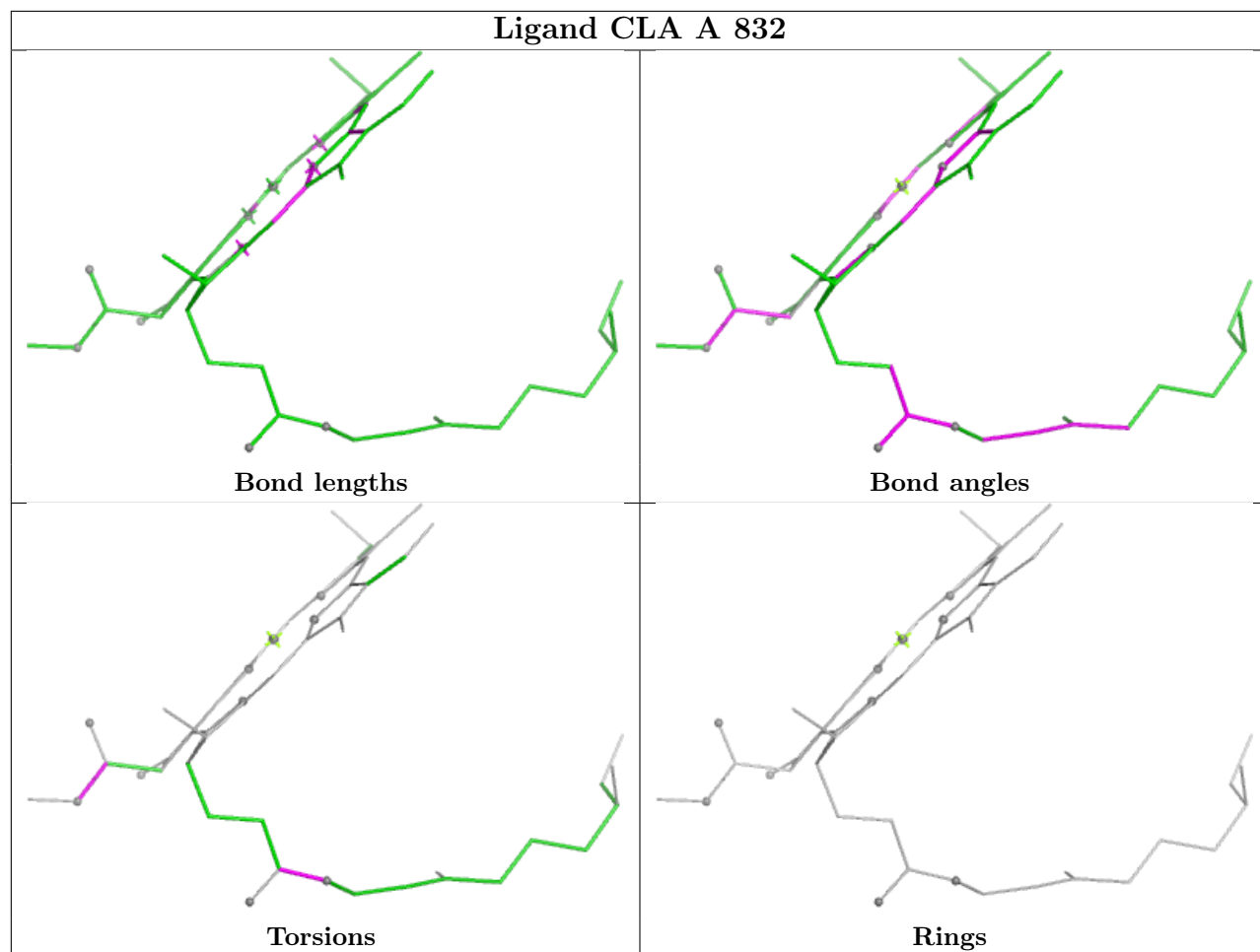
Ligand LMT G 201



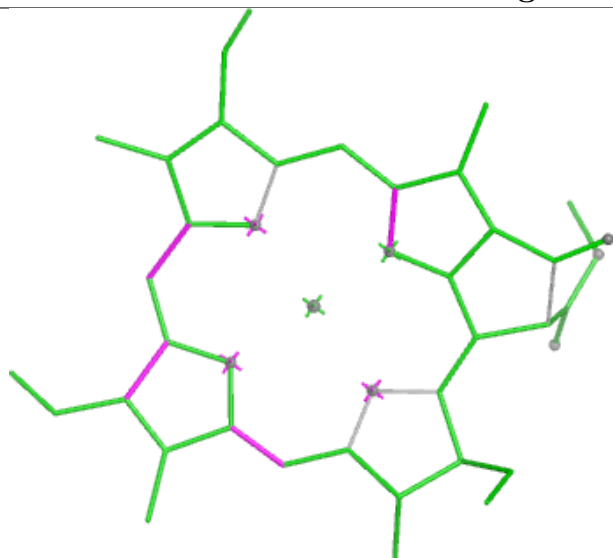


Ligand CHL 4 607

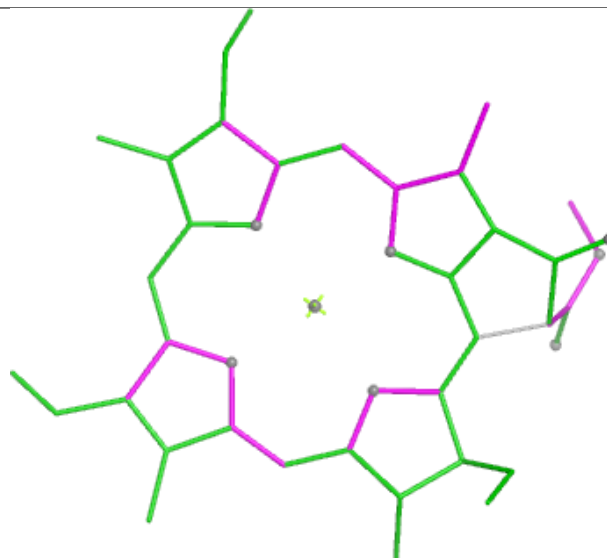




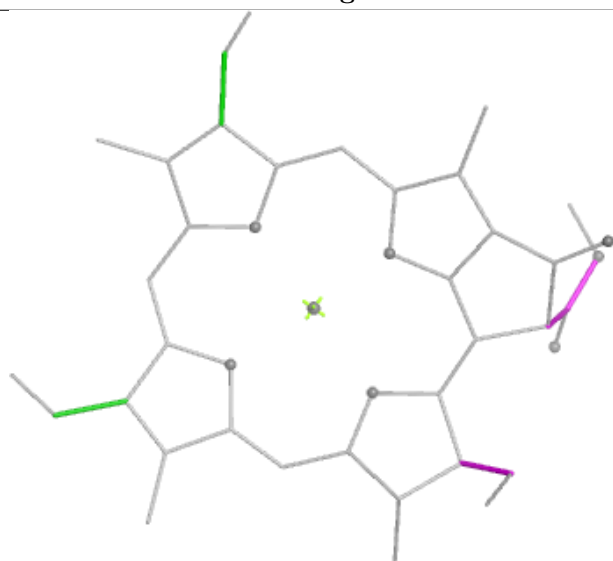
Ligand CLA J 102



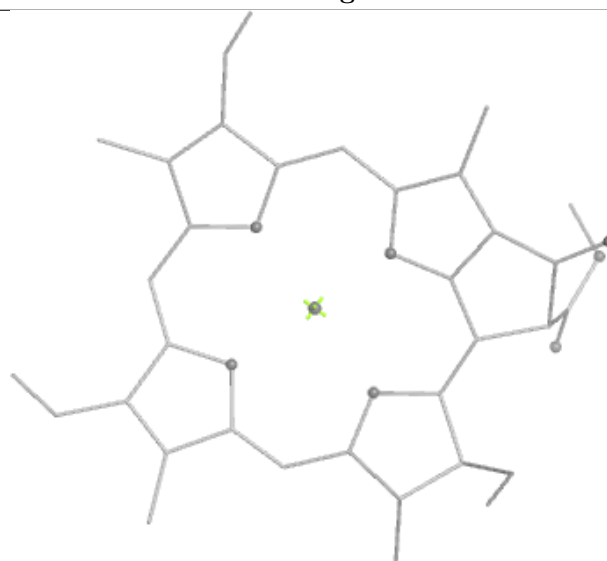
Bond lengths



Bond angles

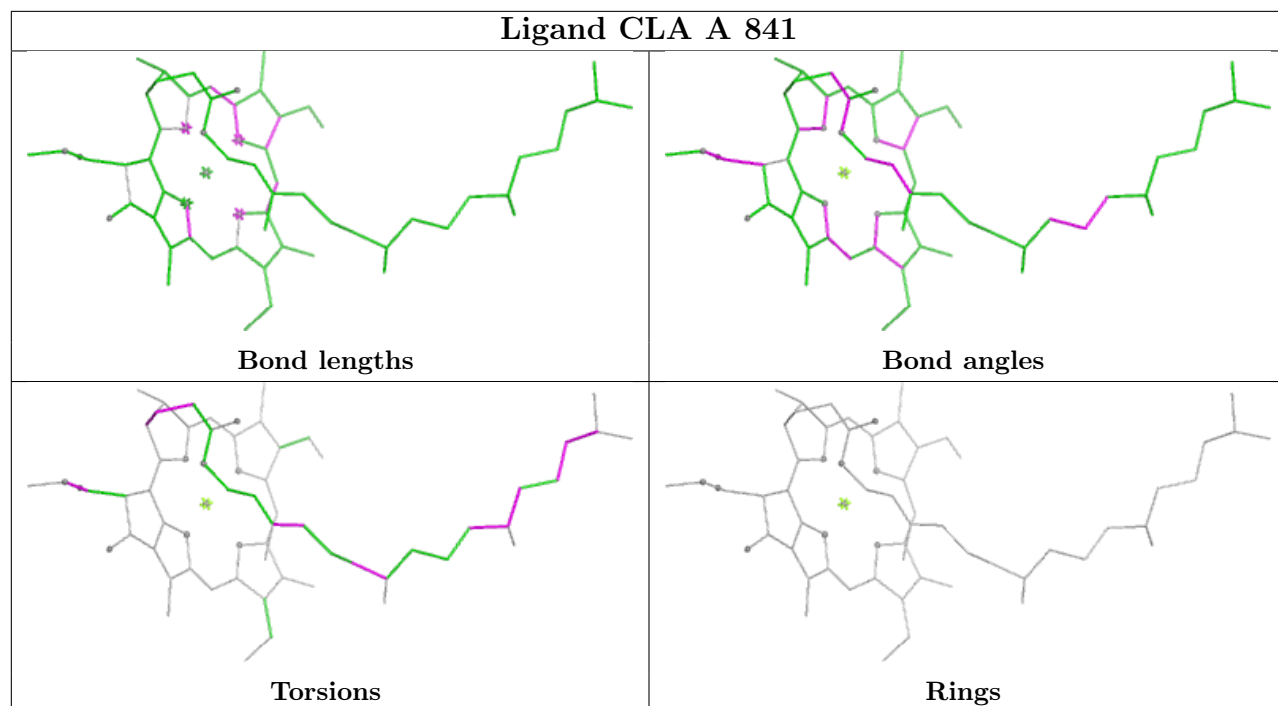


Torsions

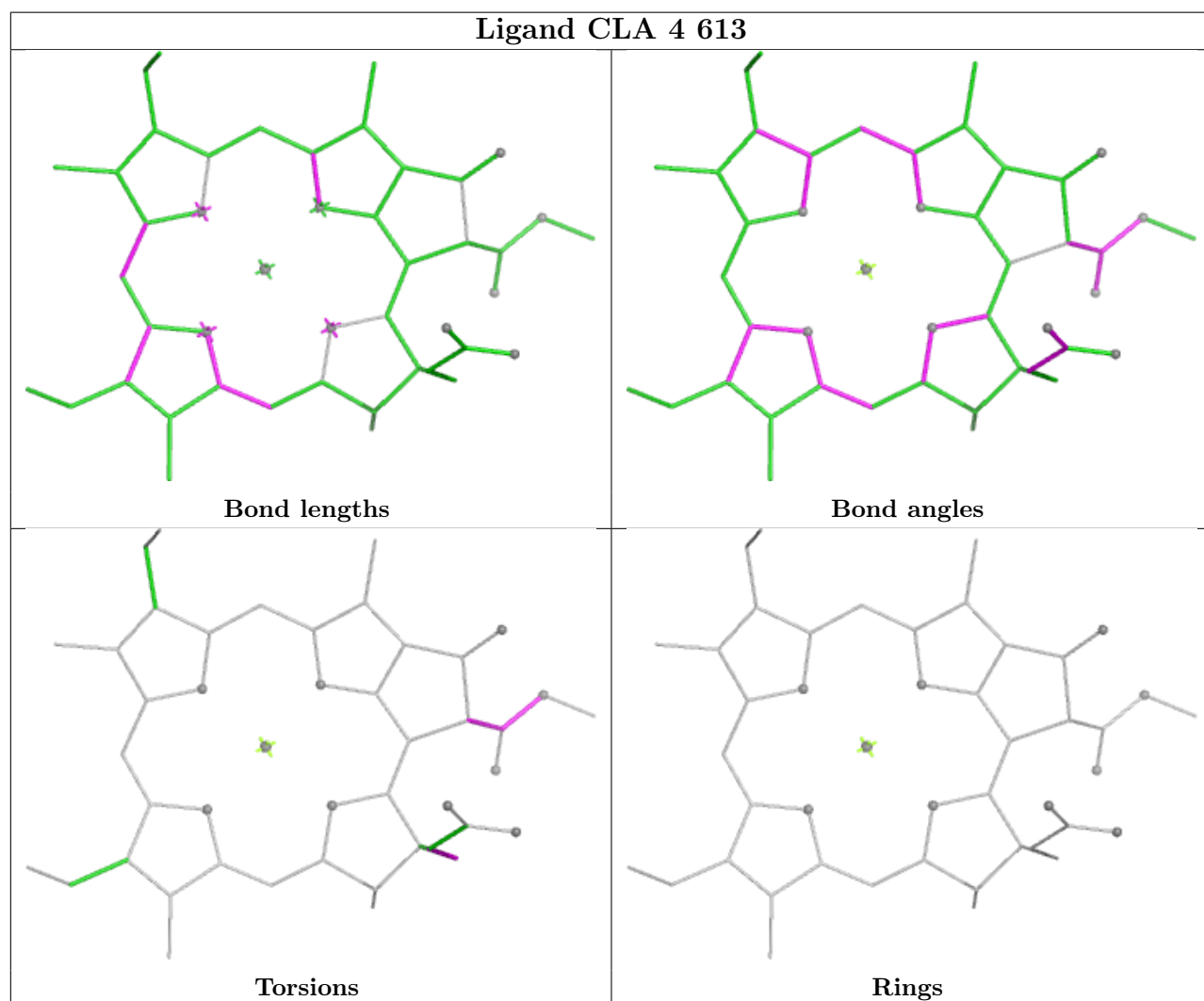


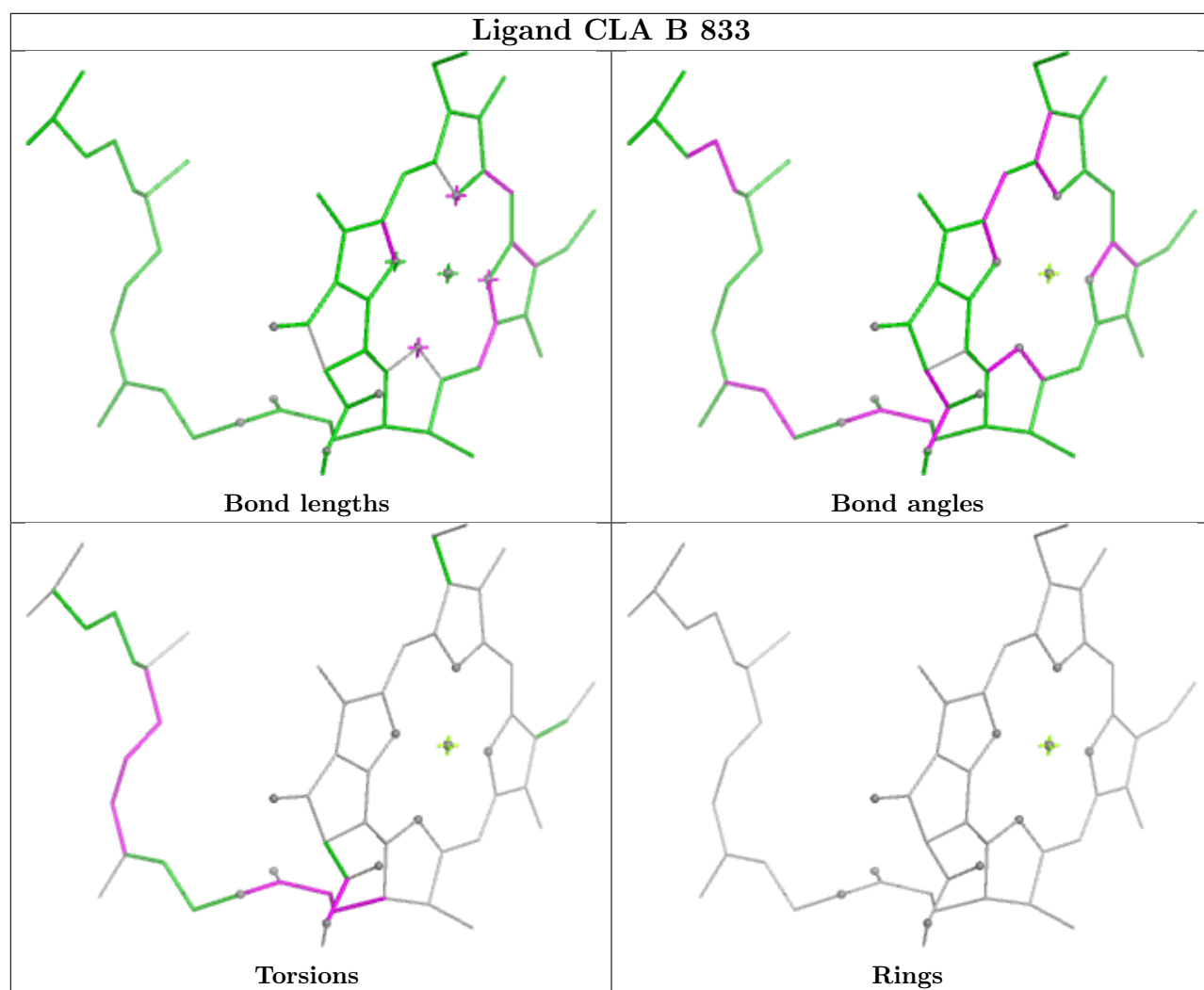
Rings

Ligand CLA A 841

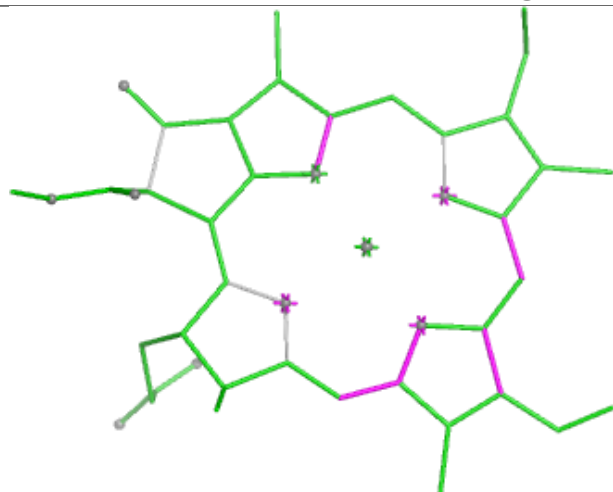


Ligand CLA 4 613

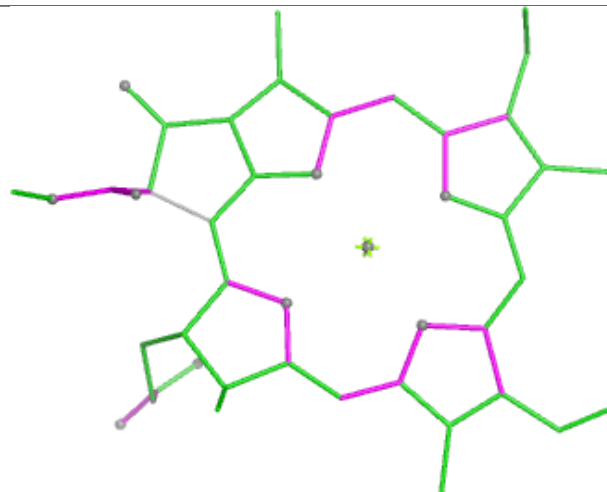




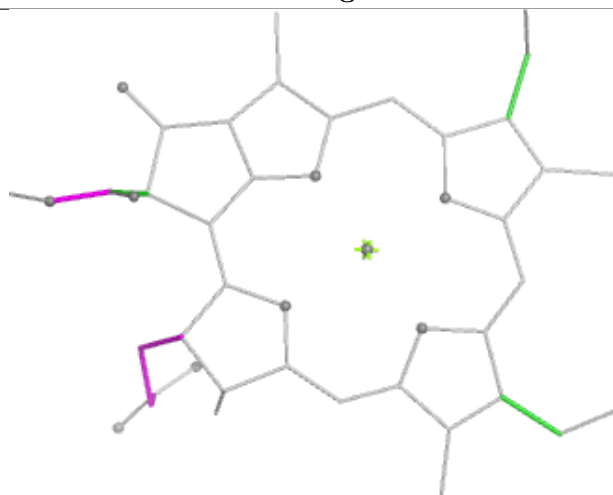
Ligand CLA 3 607



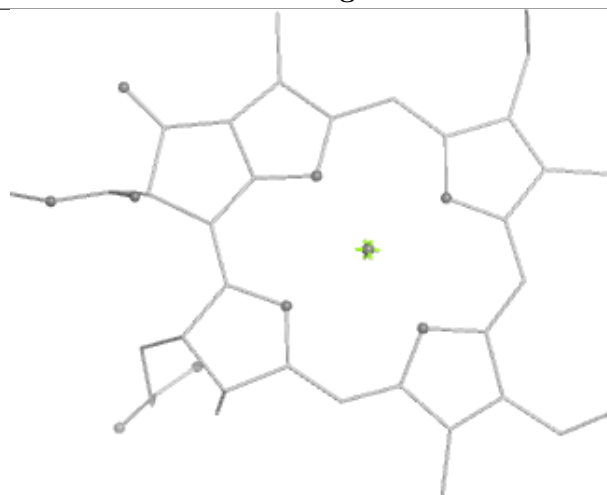
Bond lengths



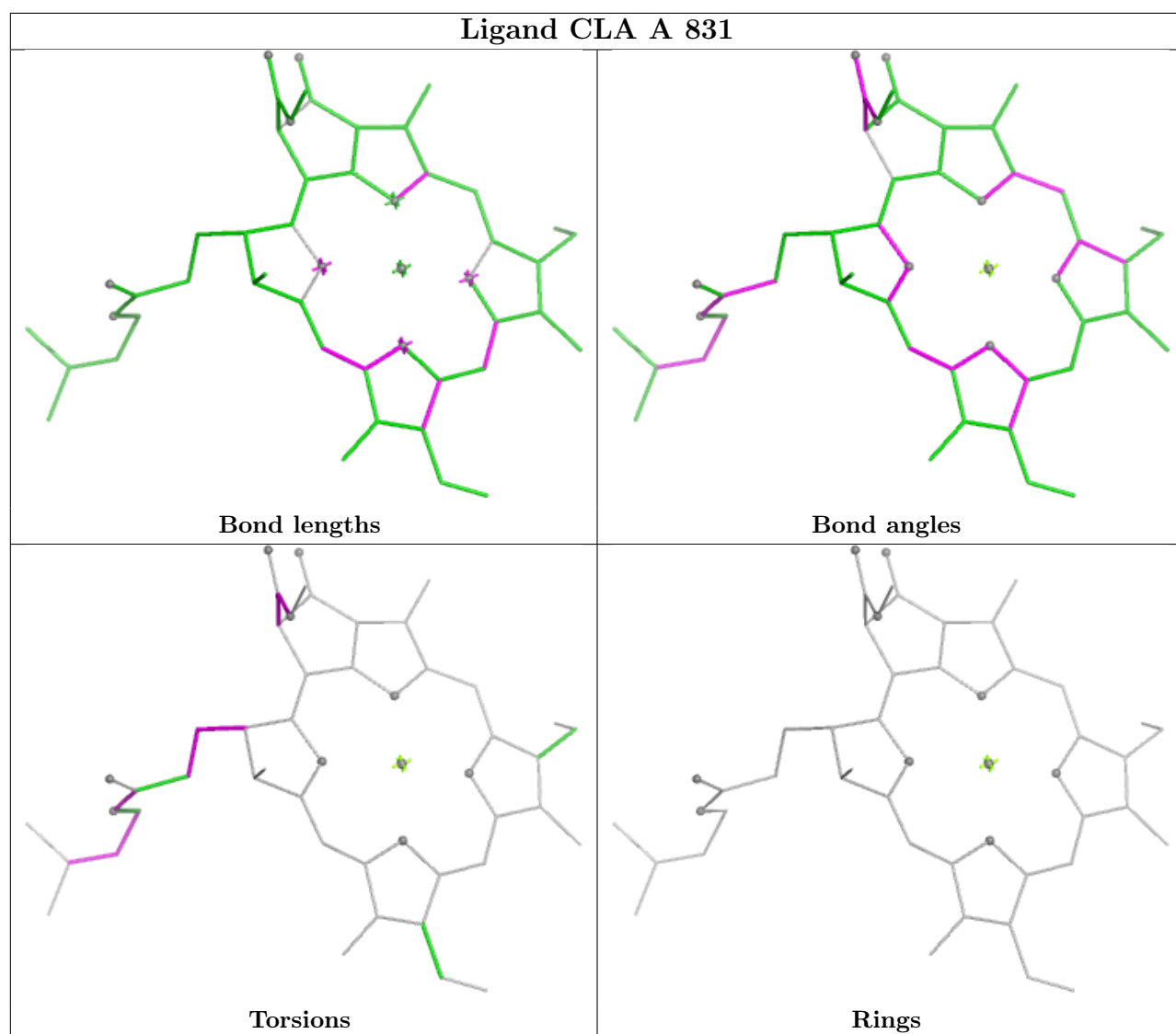
Bond angles



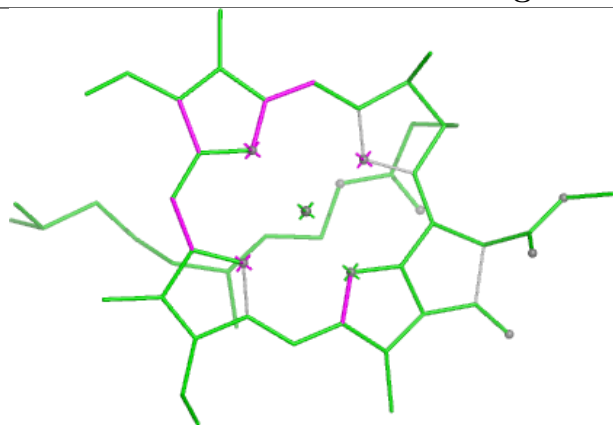
Torsions



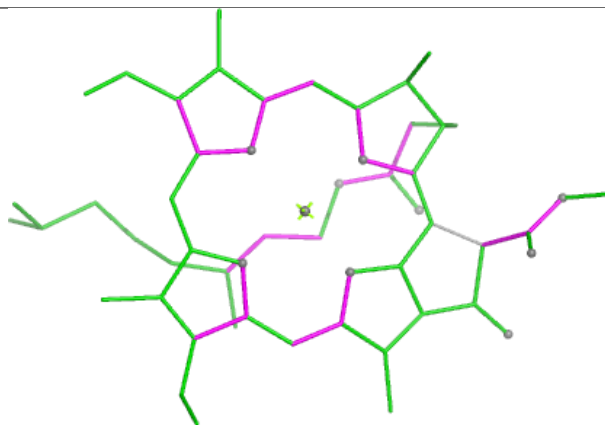
Rings



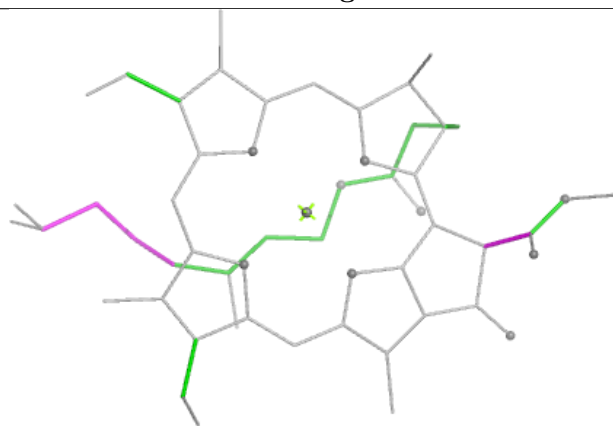
Ligand CLA A 838



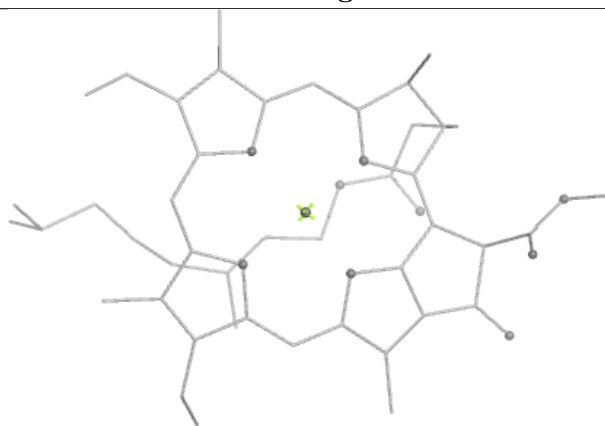
Bond lengths



Bond angles

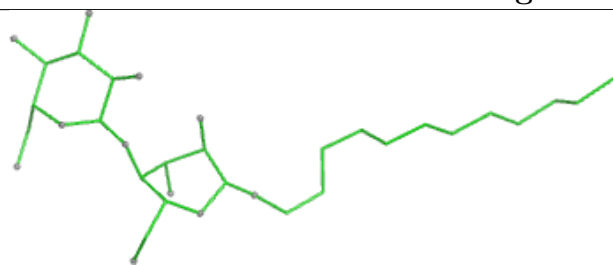


Torsions

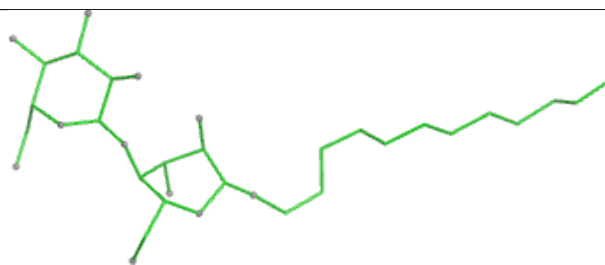


Rings

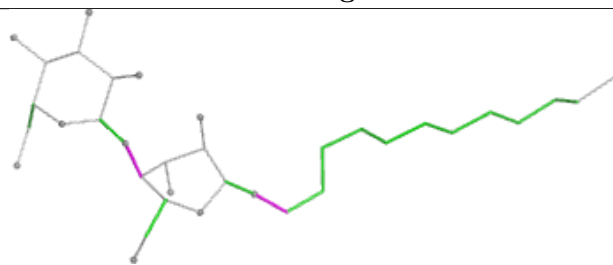
Ligand LMT 4 620



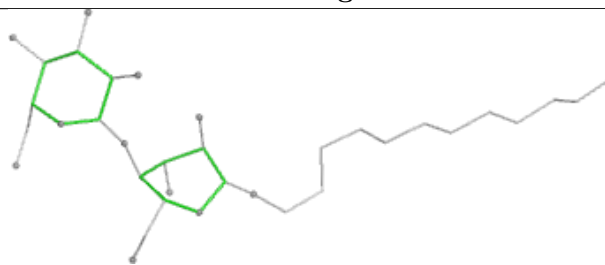
Bond lengths



Bond angles

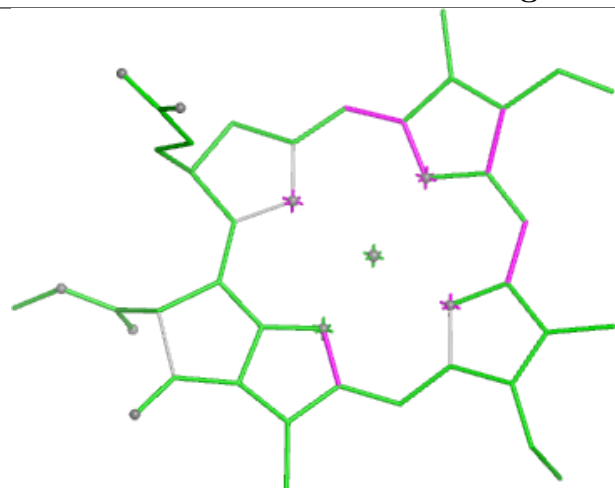


Torsions

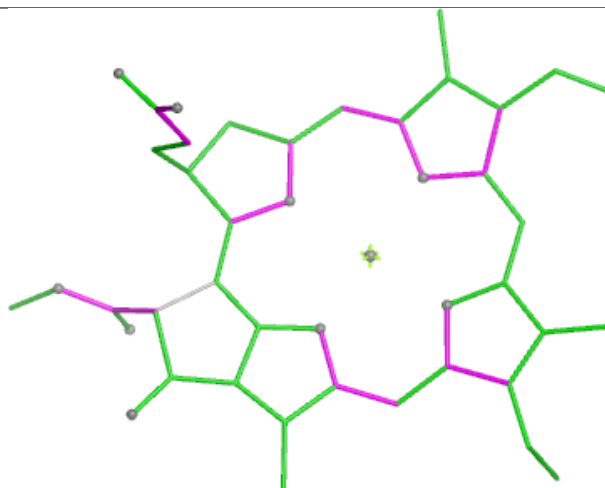


Rings

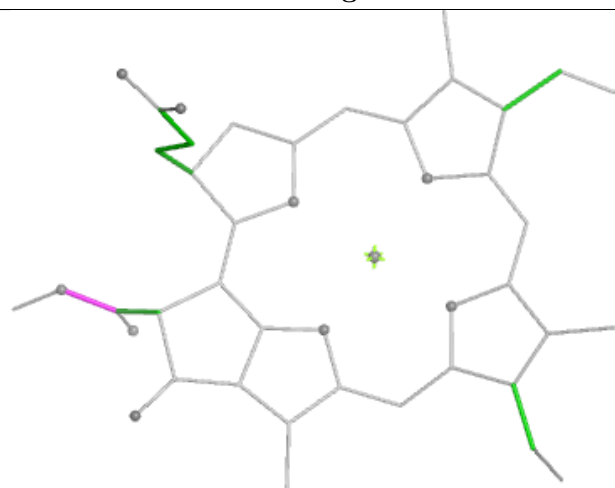
Ligand CLA 3 608



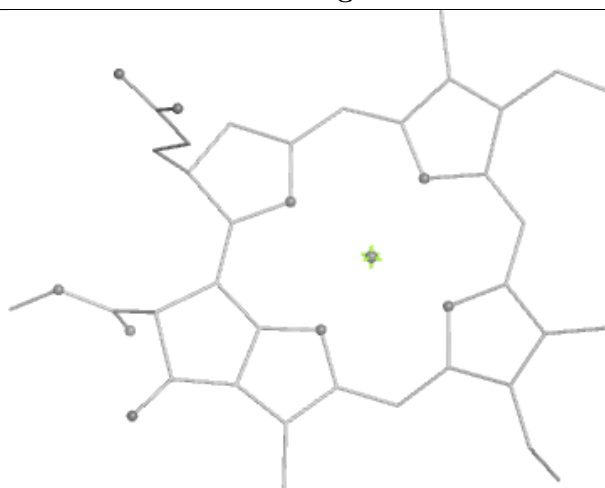
Bond lengths



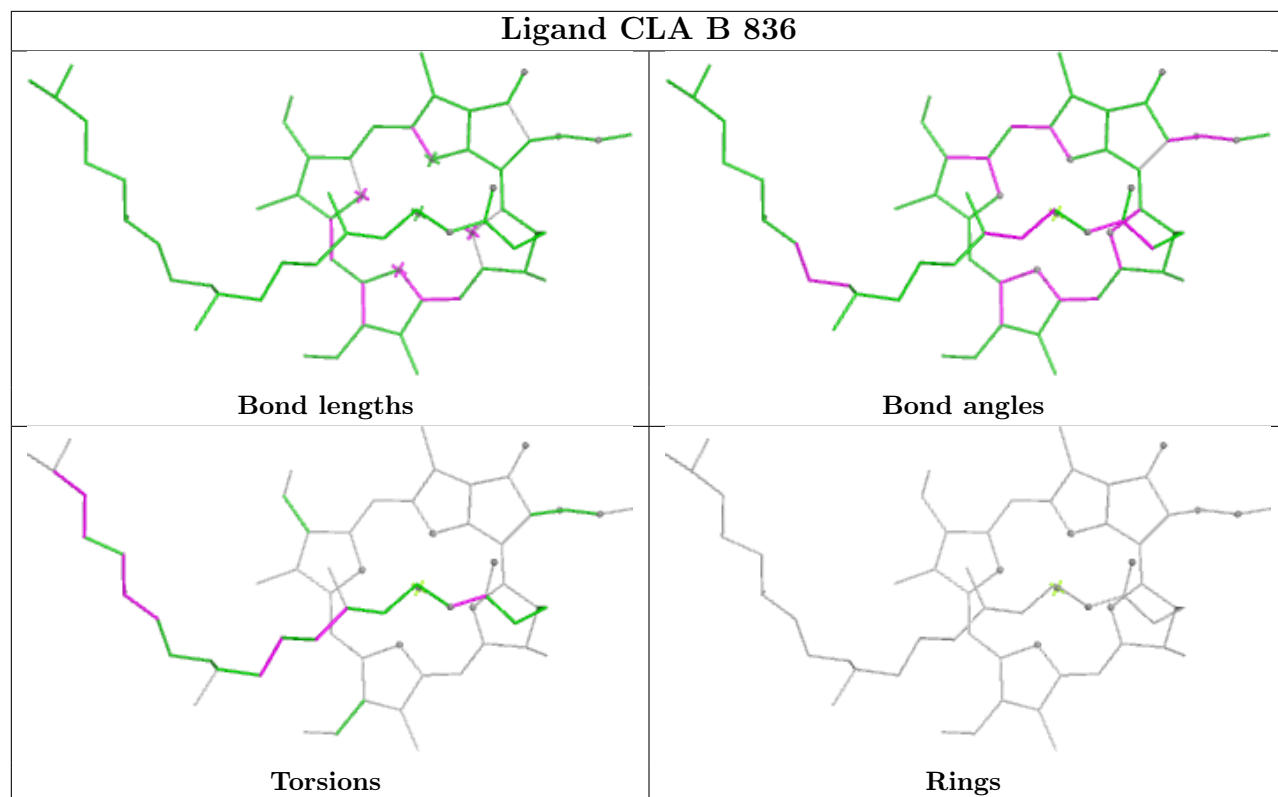
Bond angles

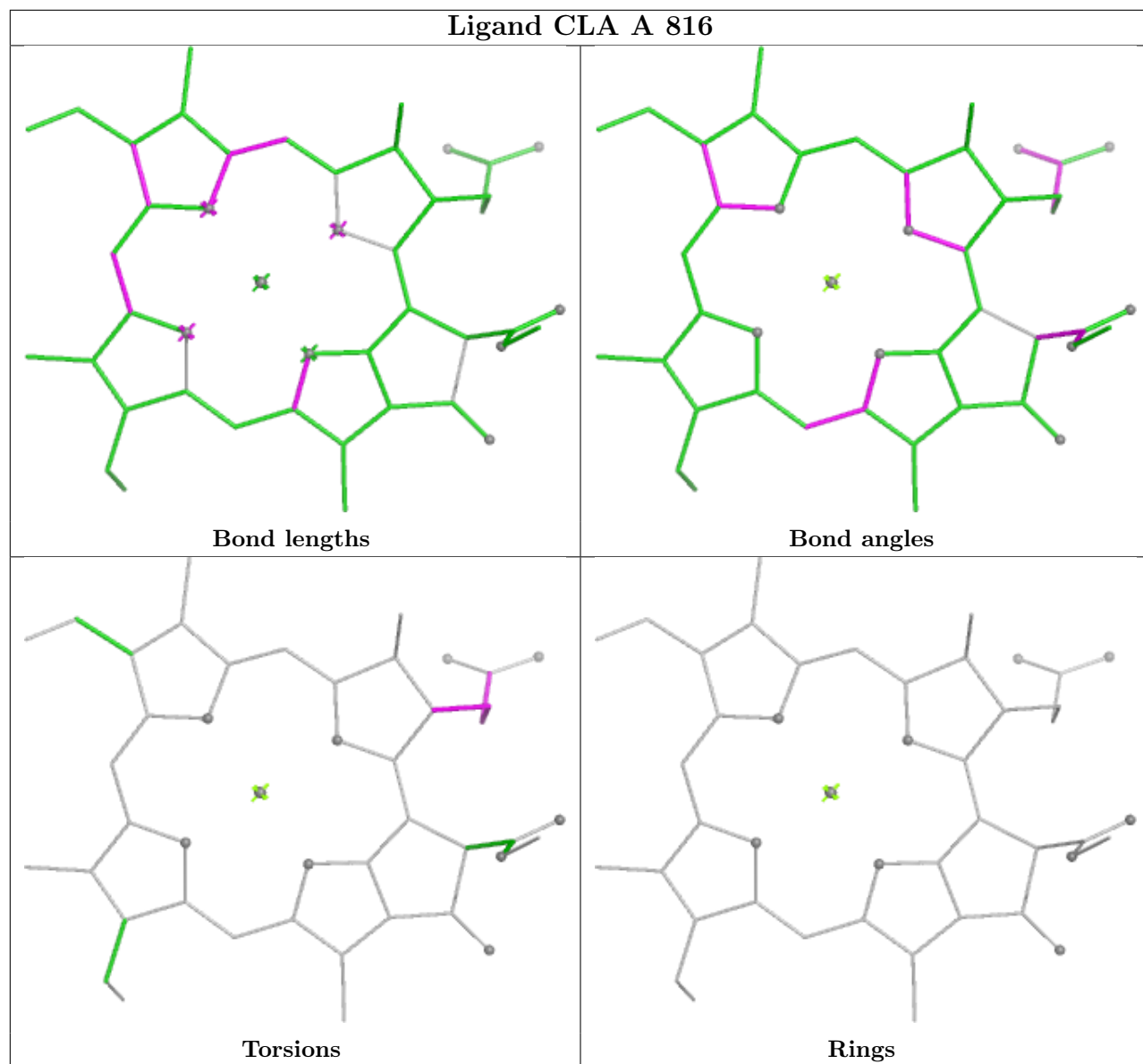


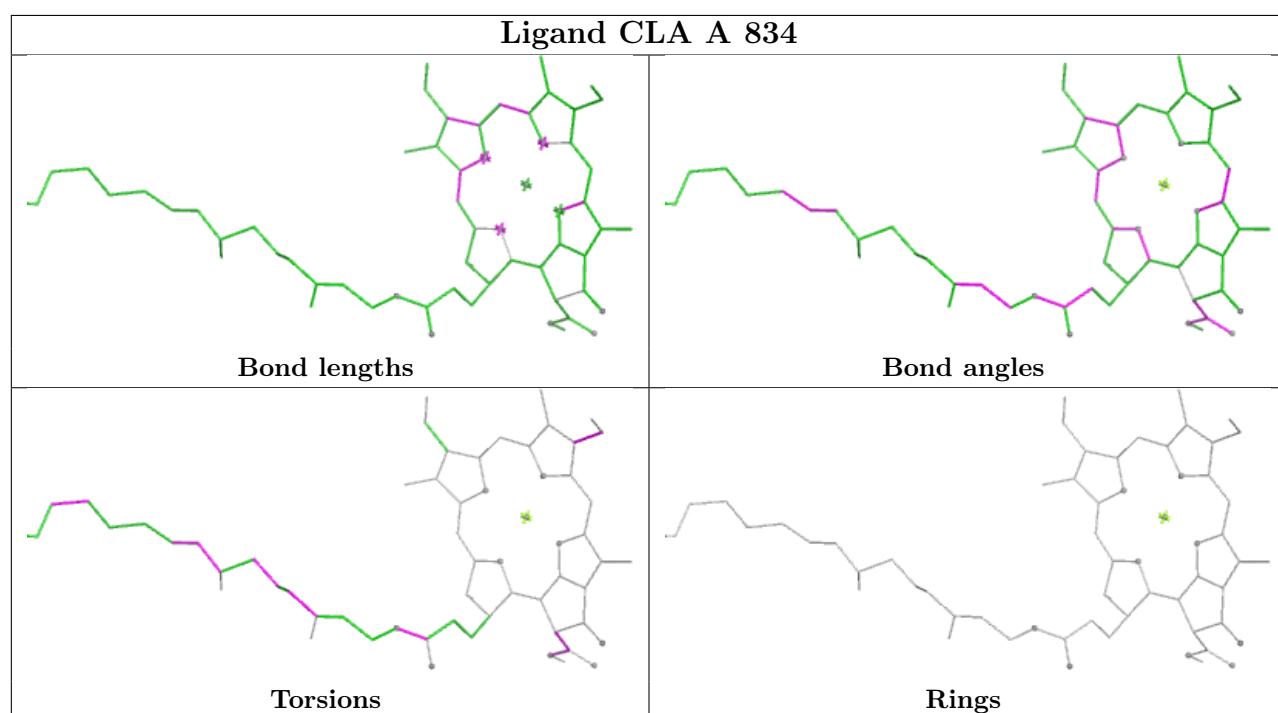
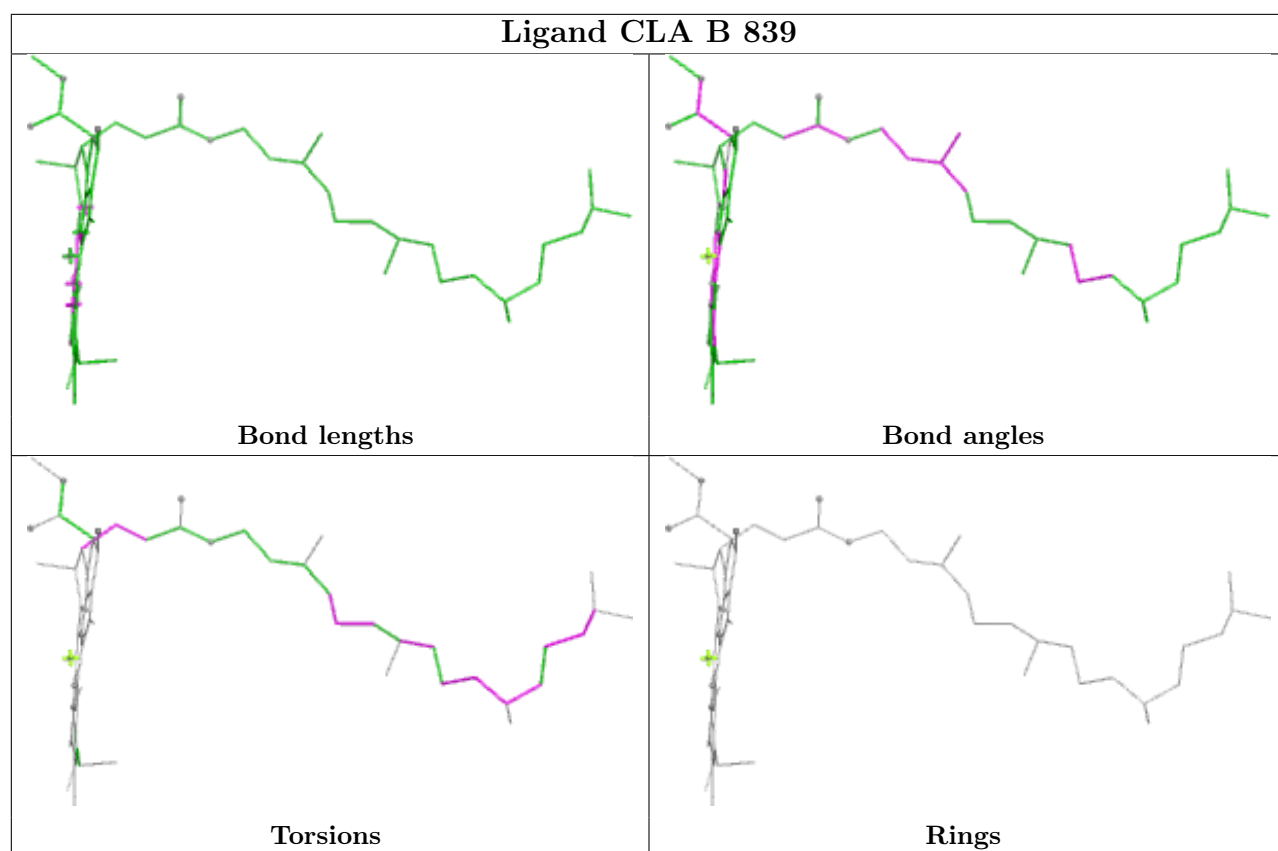
Torsions

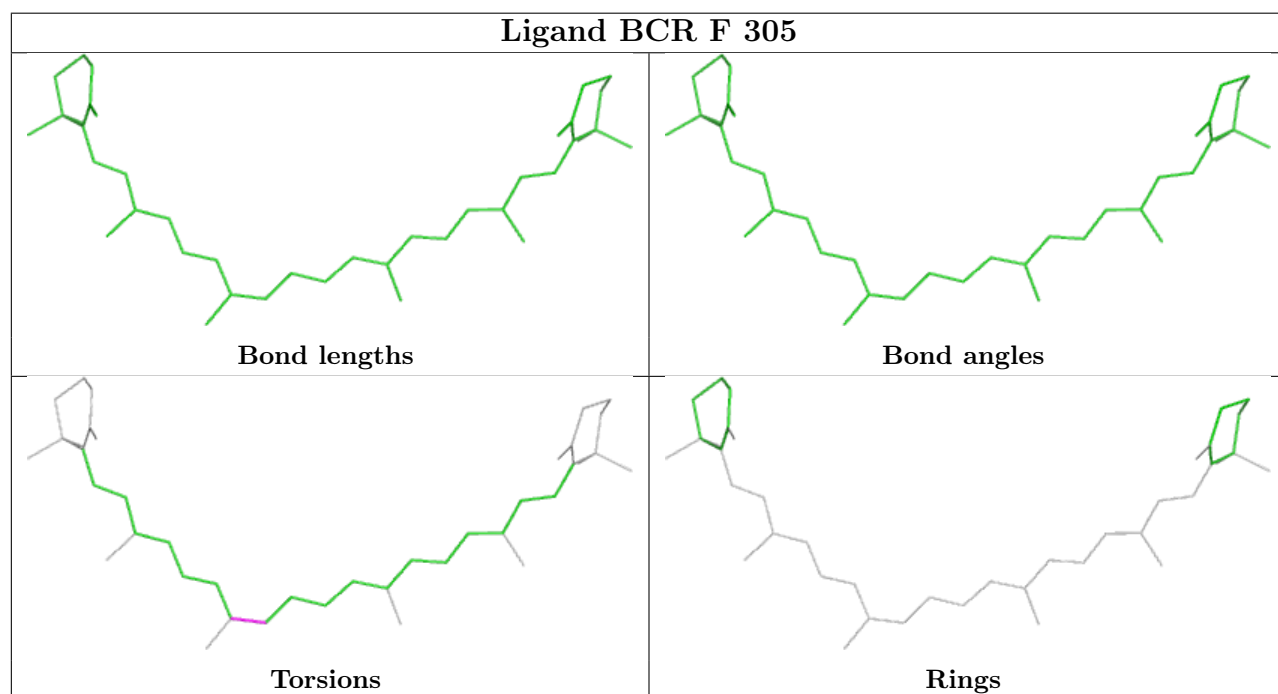
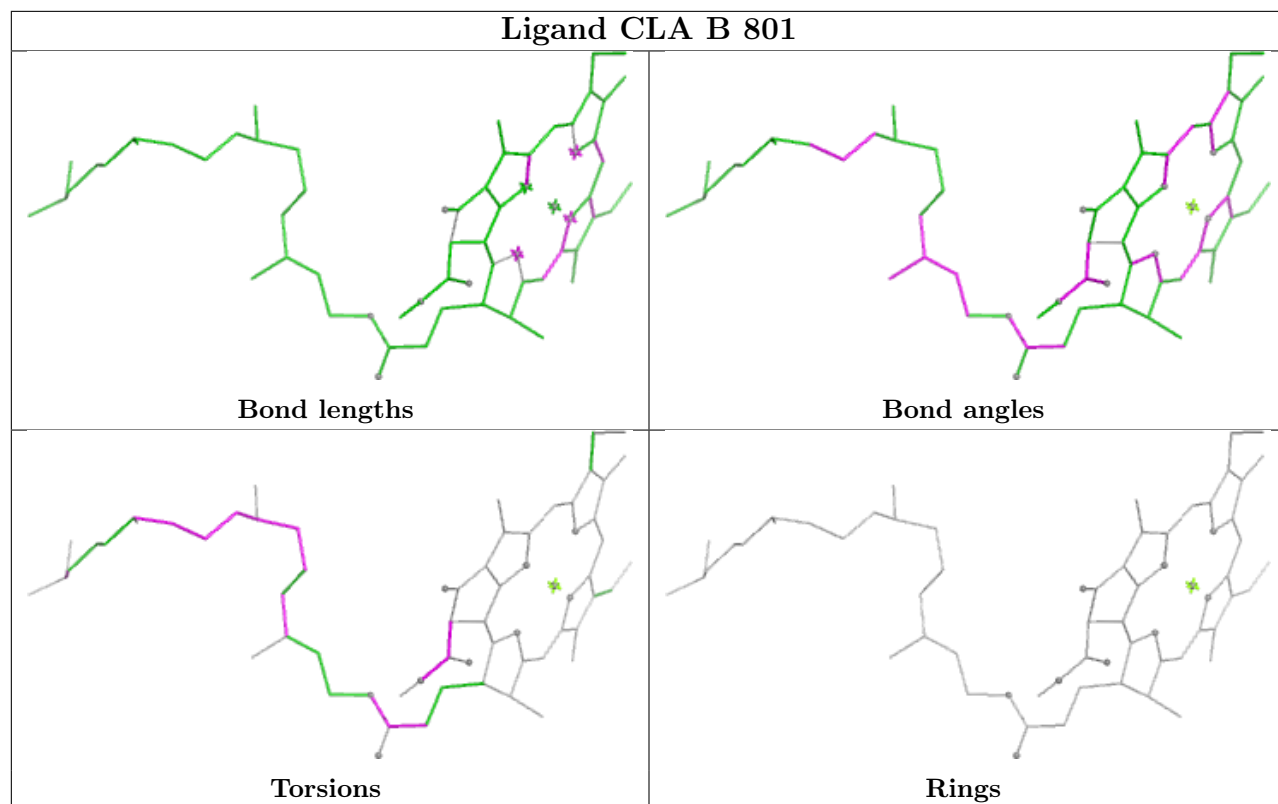


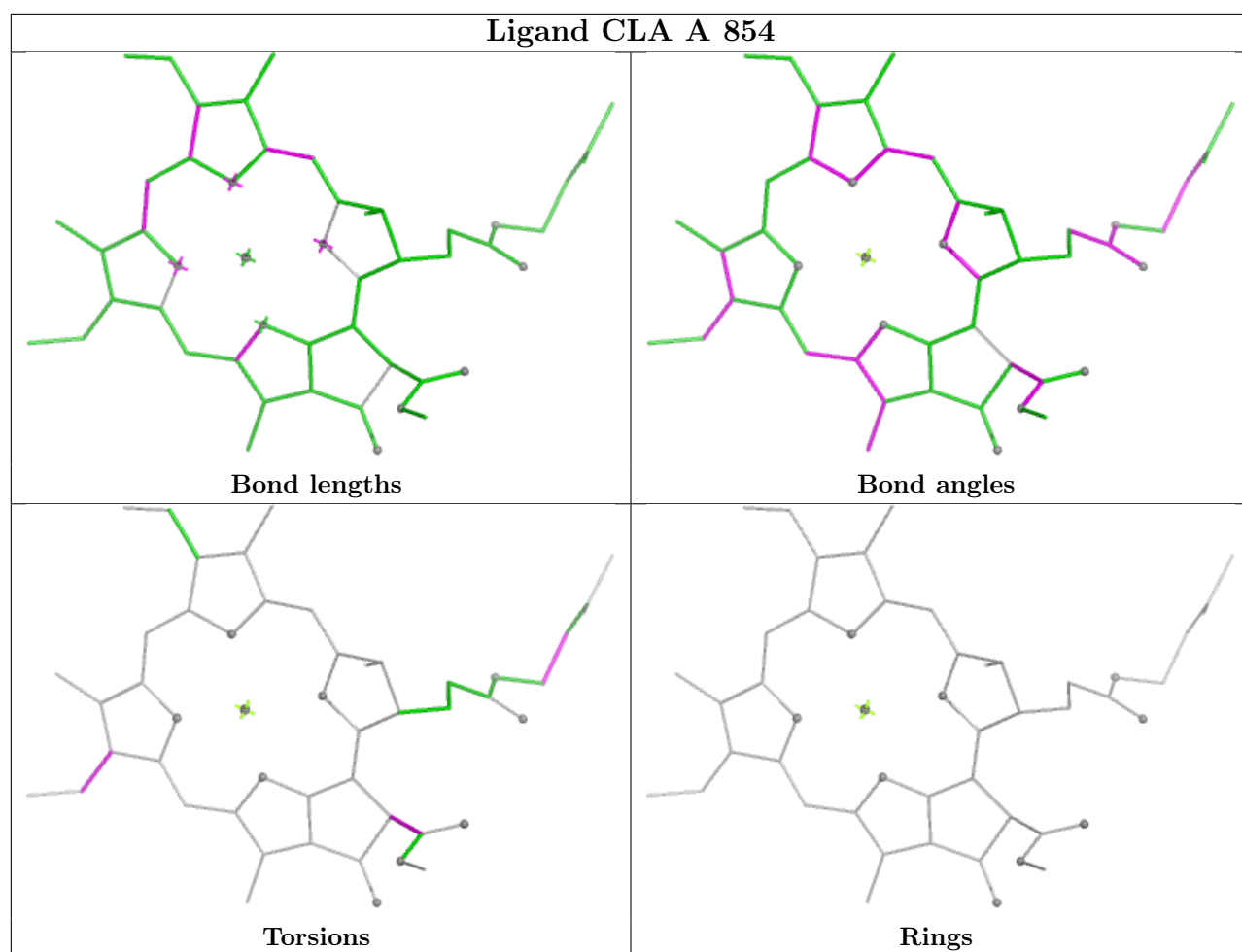
Rings

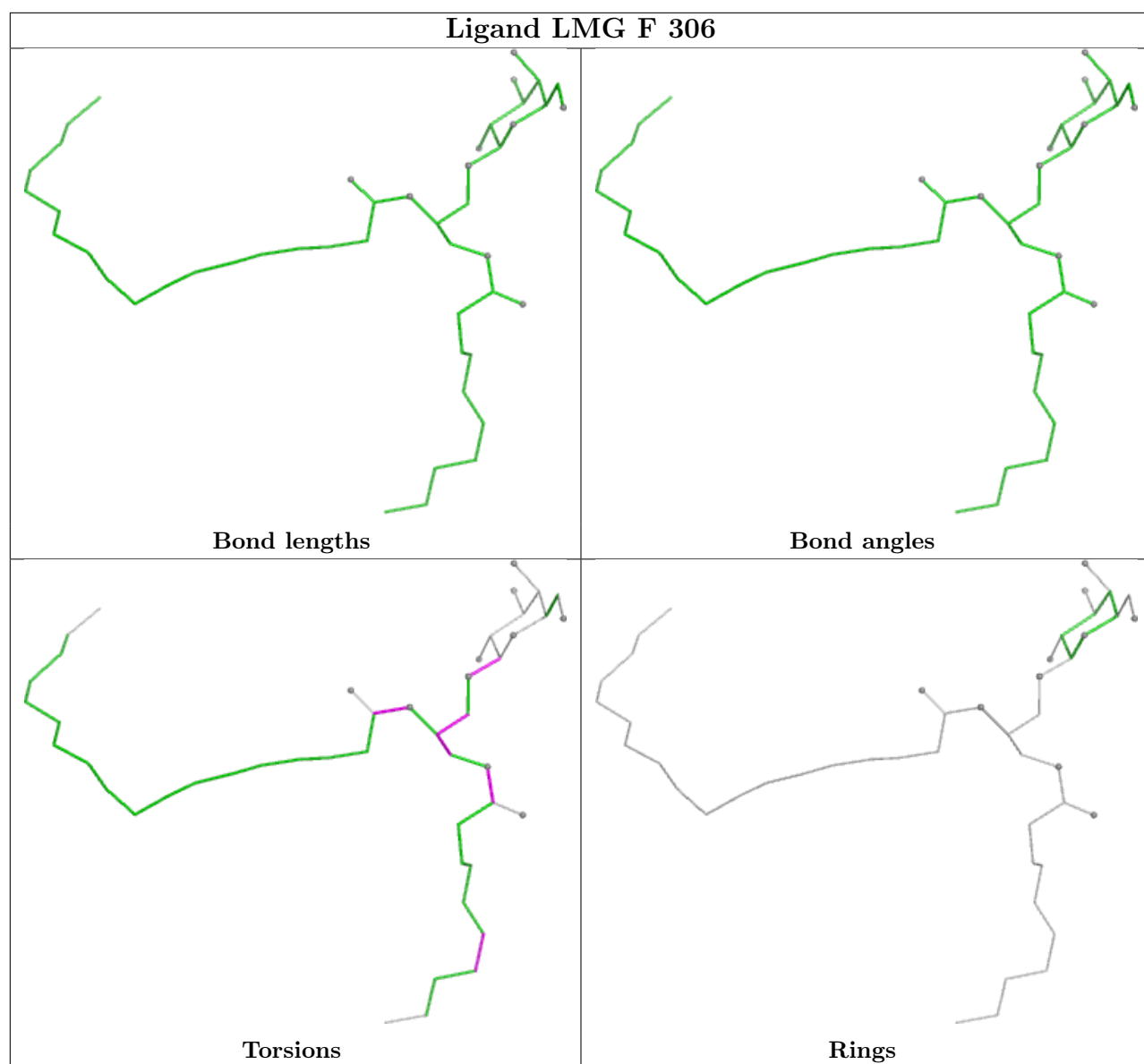




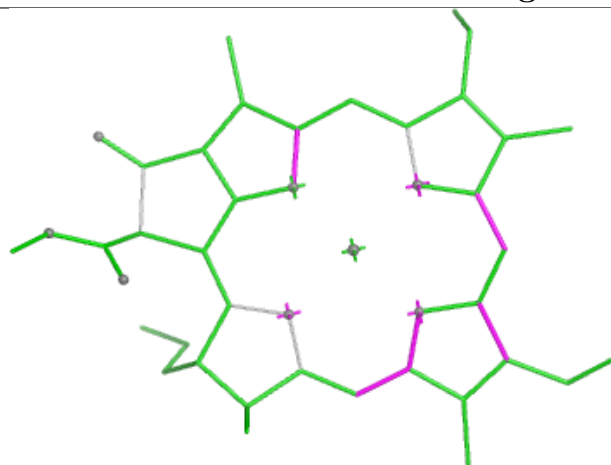




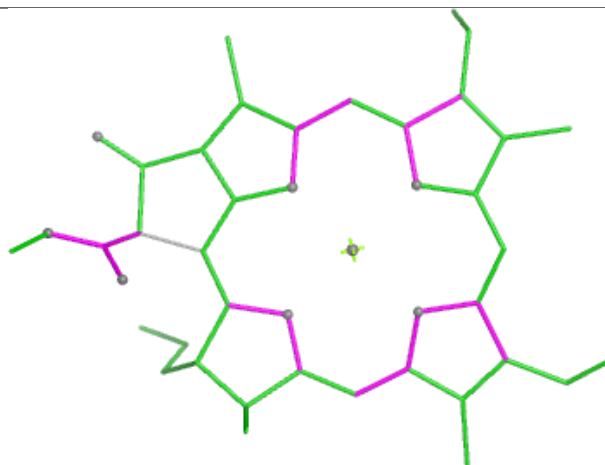




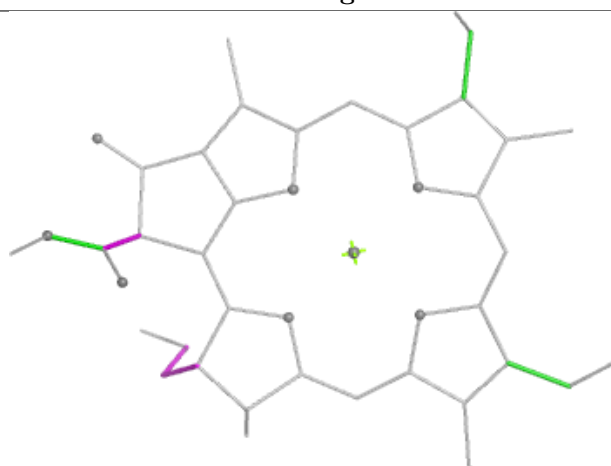
Ligand CLA 2 613



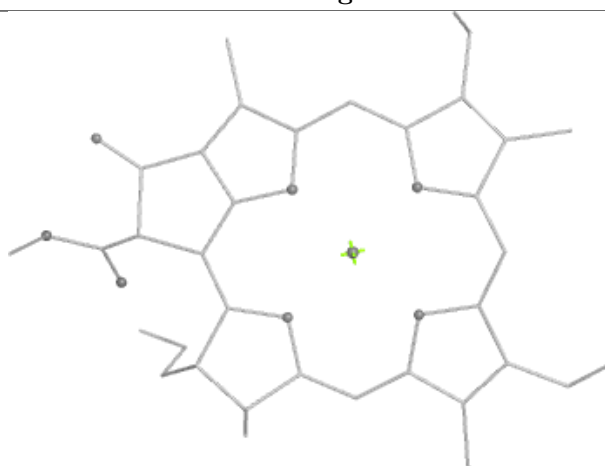
Bond lengths



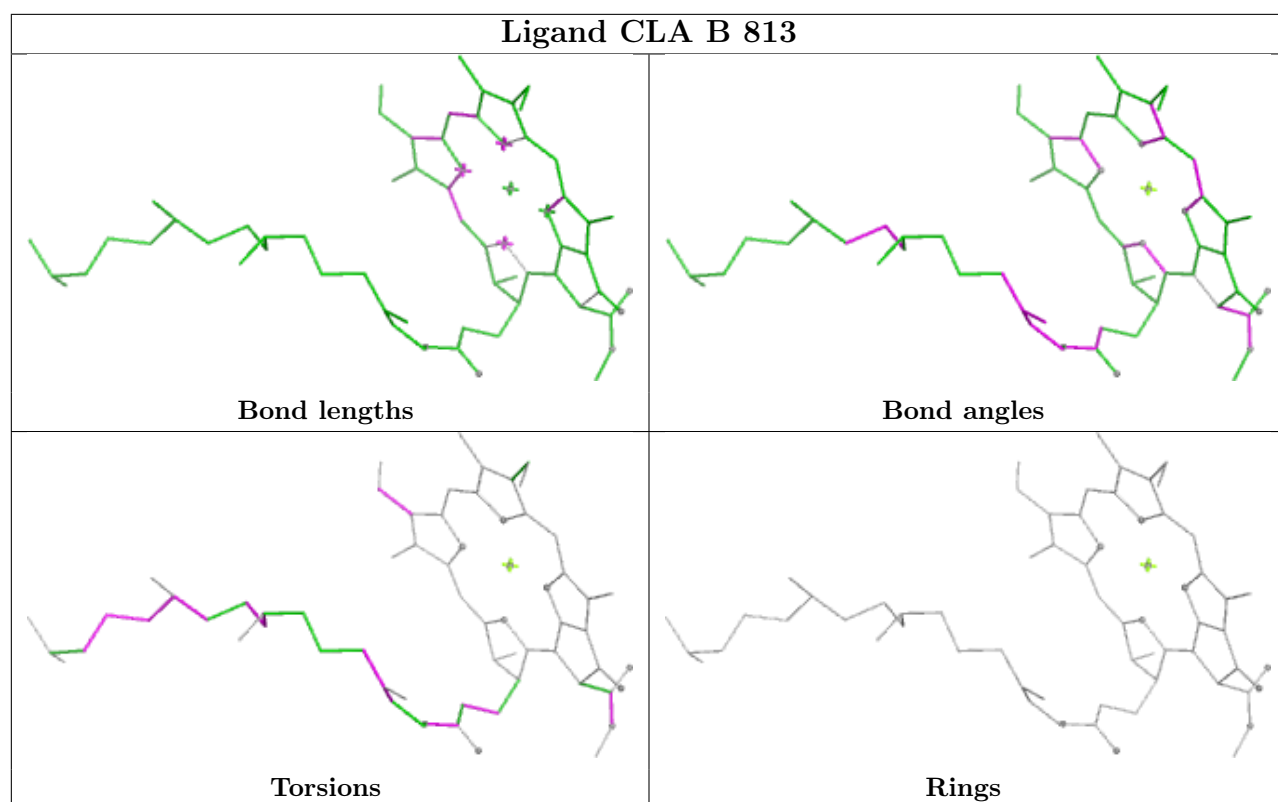
Bond angles

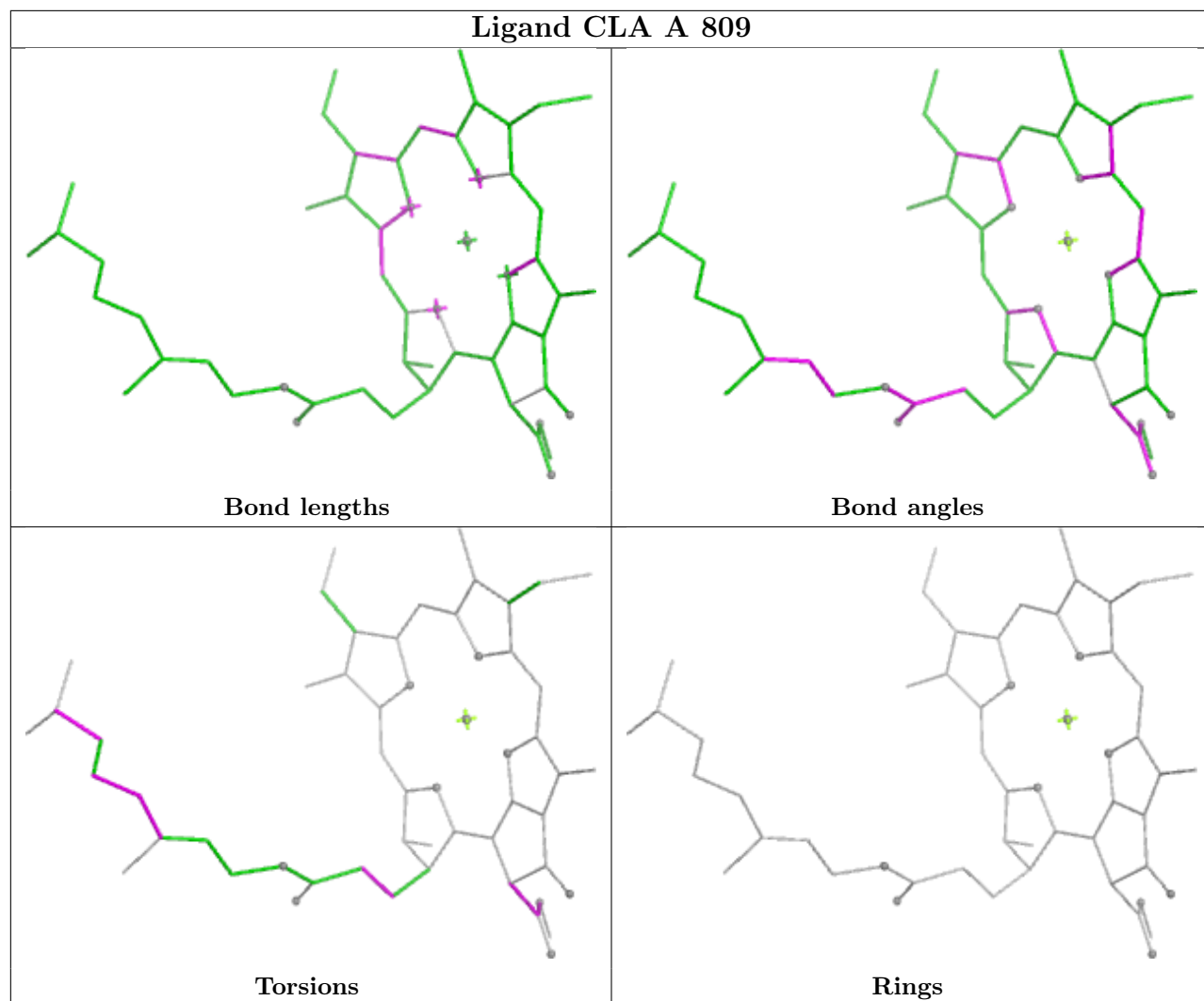


Torsions

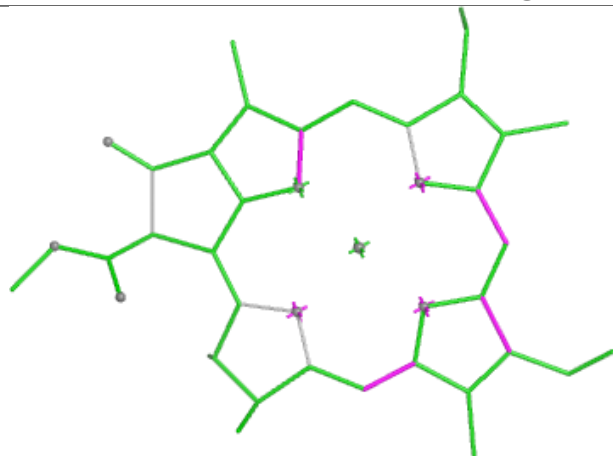


Rings

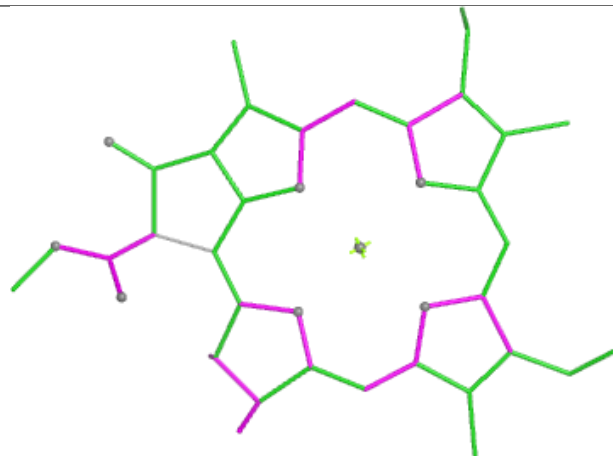




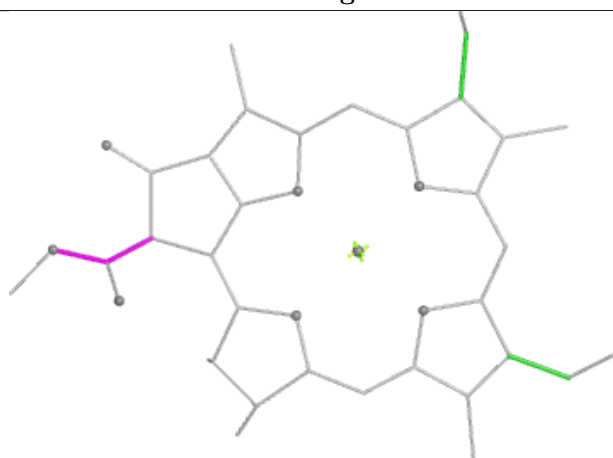
Ligand CLA 3 609



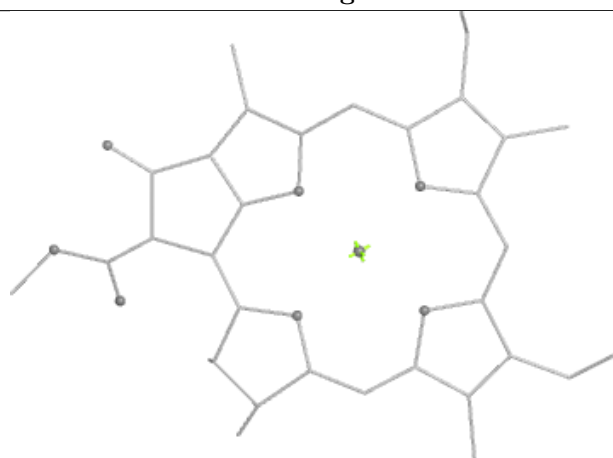
Bond lengths



Bond angles

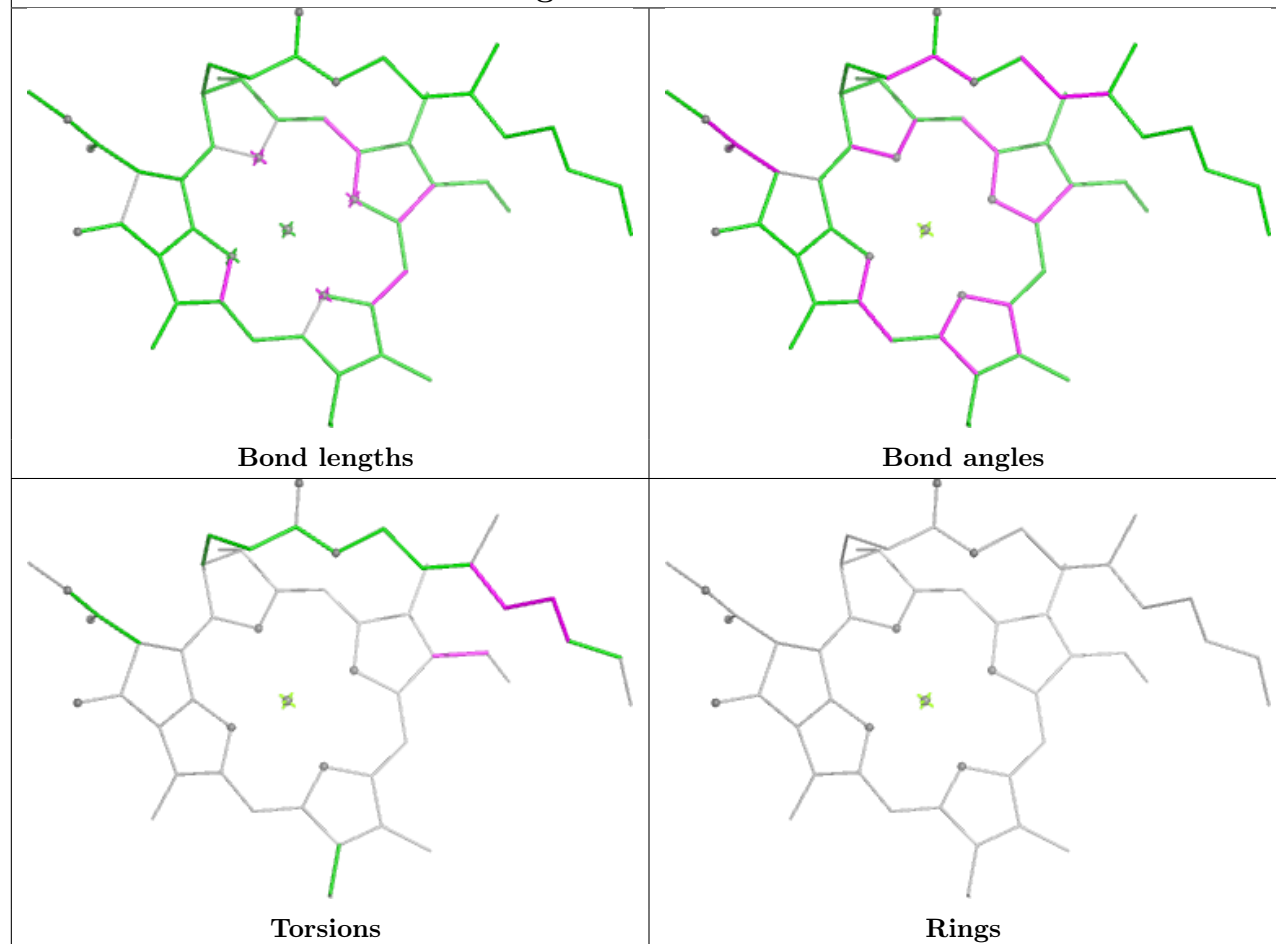


Torsions

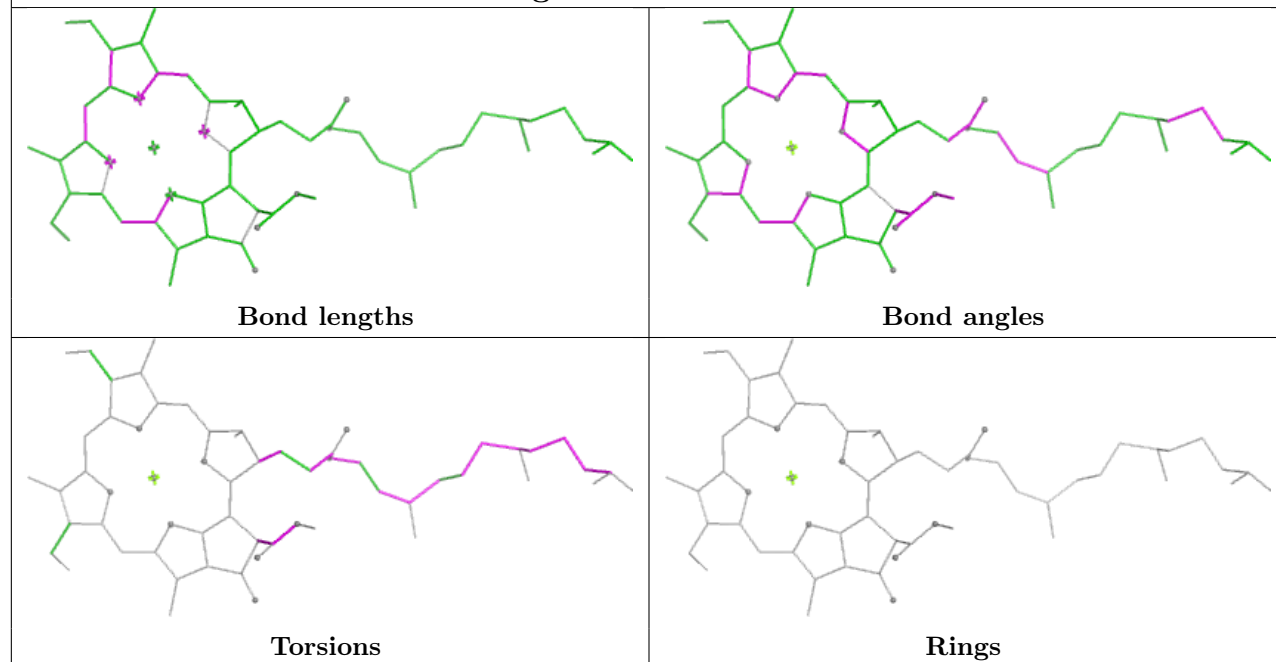


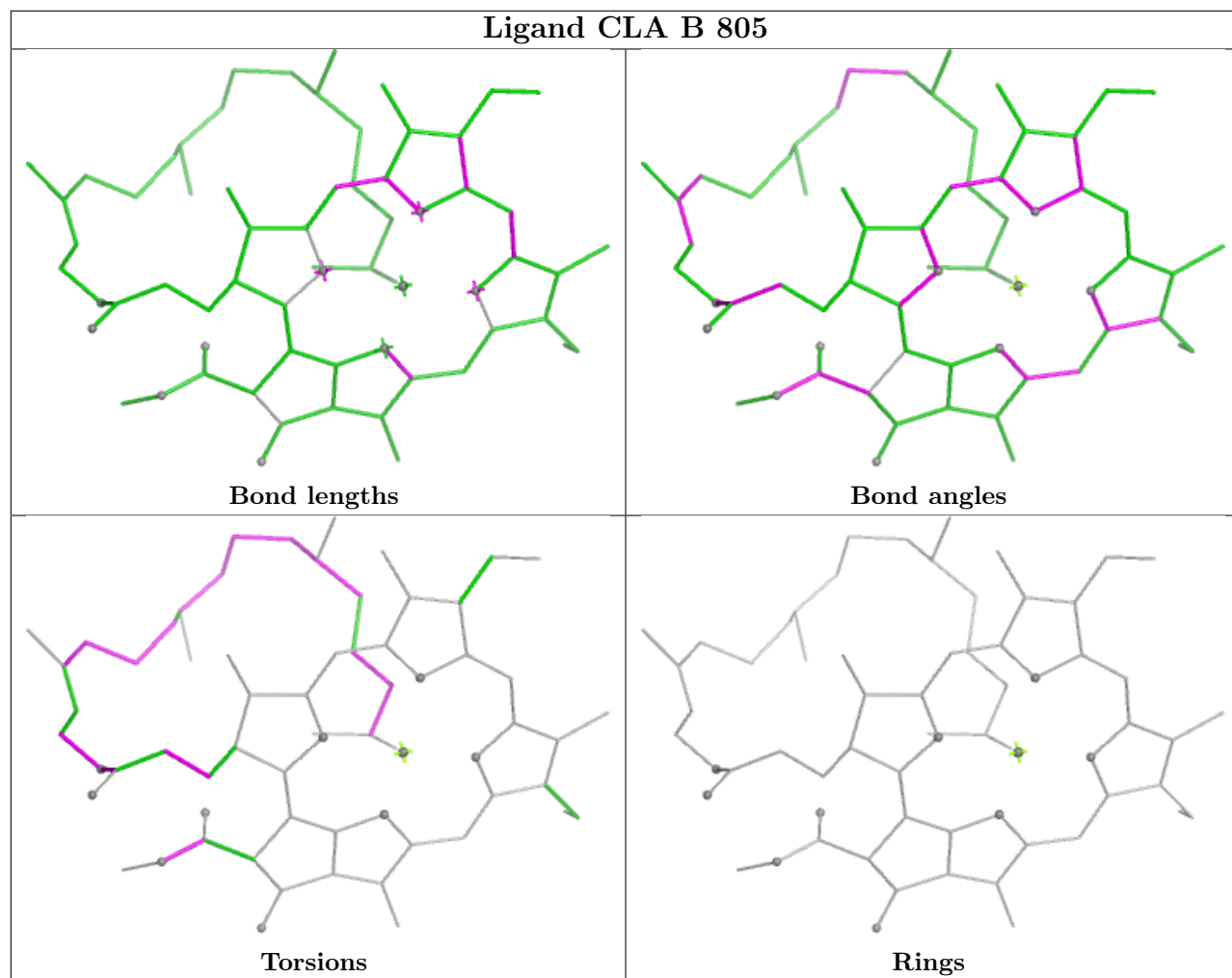
Rings

Ligand CLA 4 609

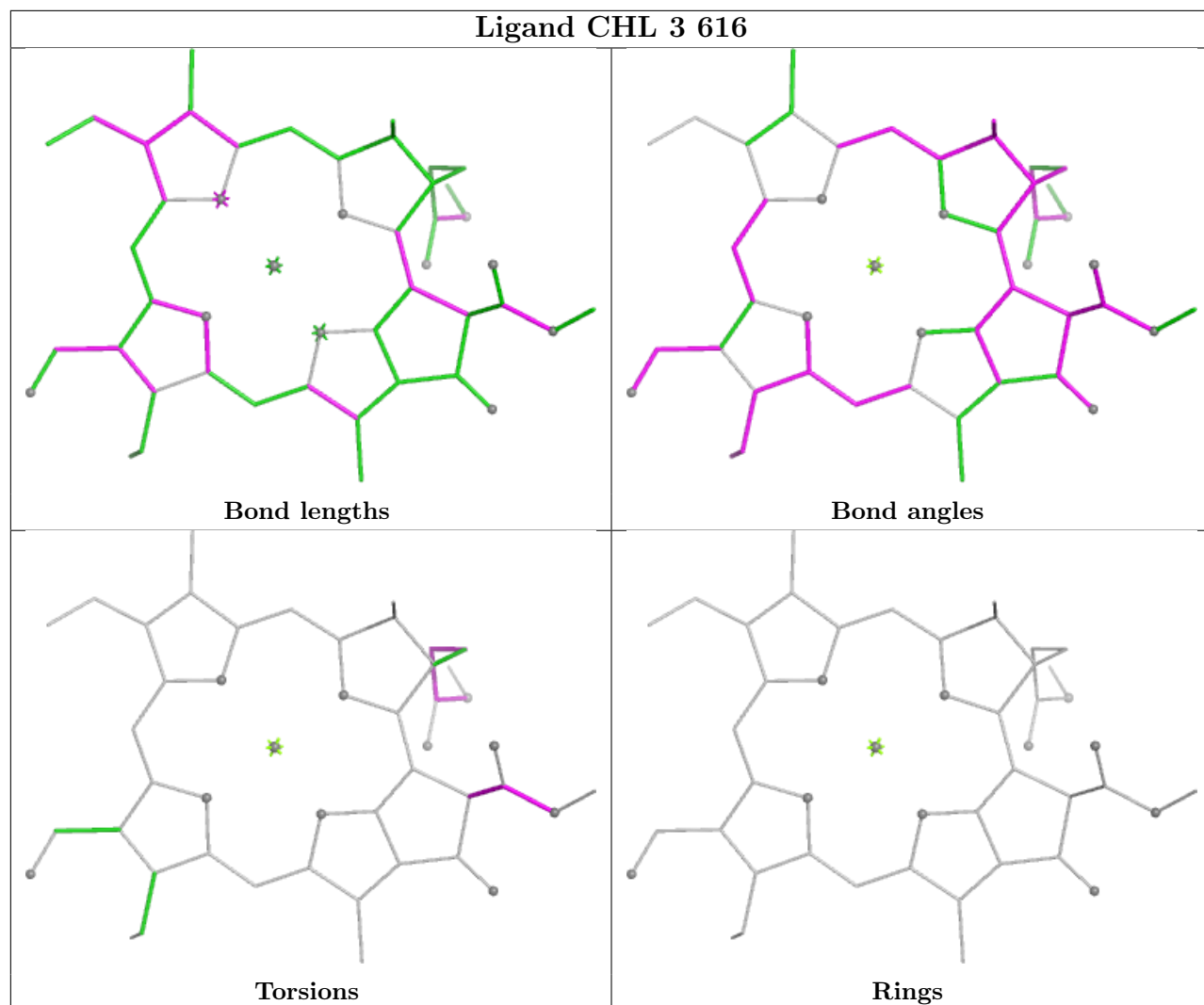


Ligand CLA B 822

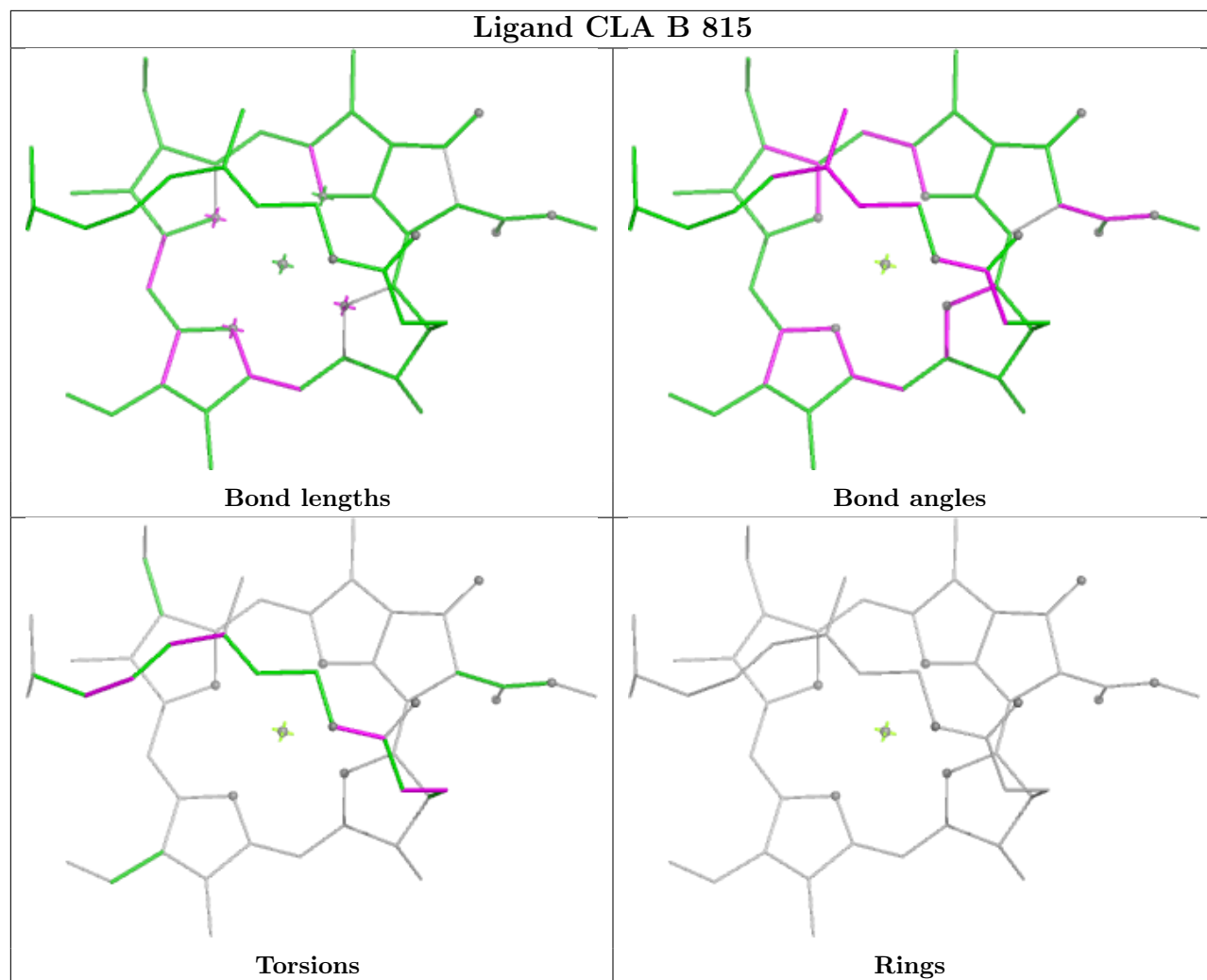


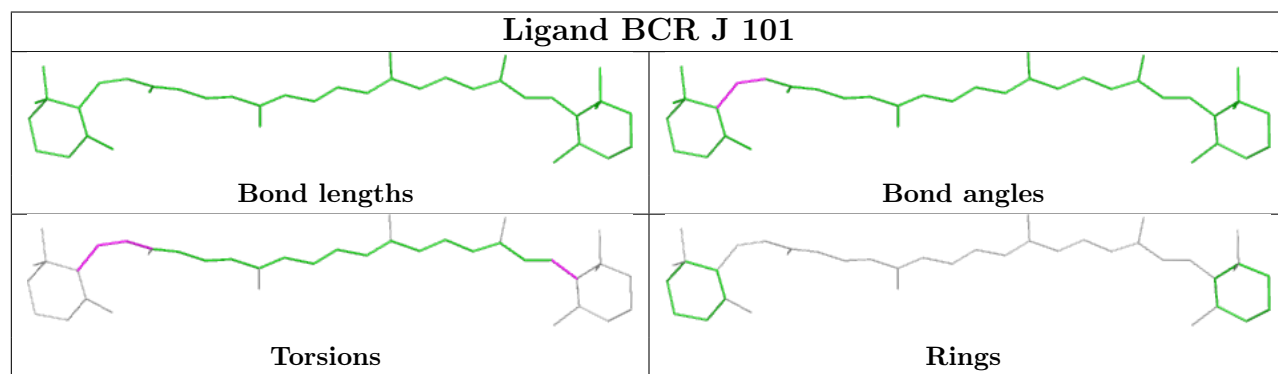
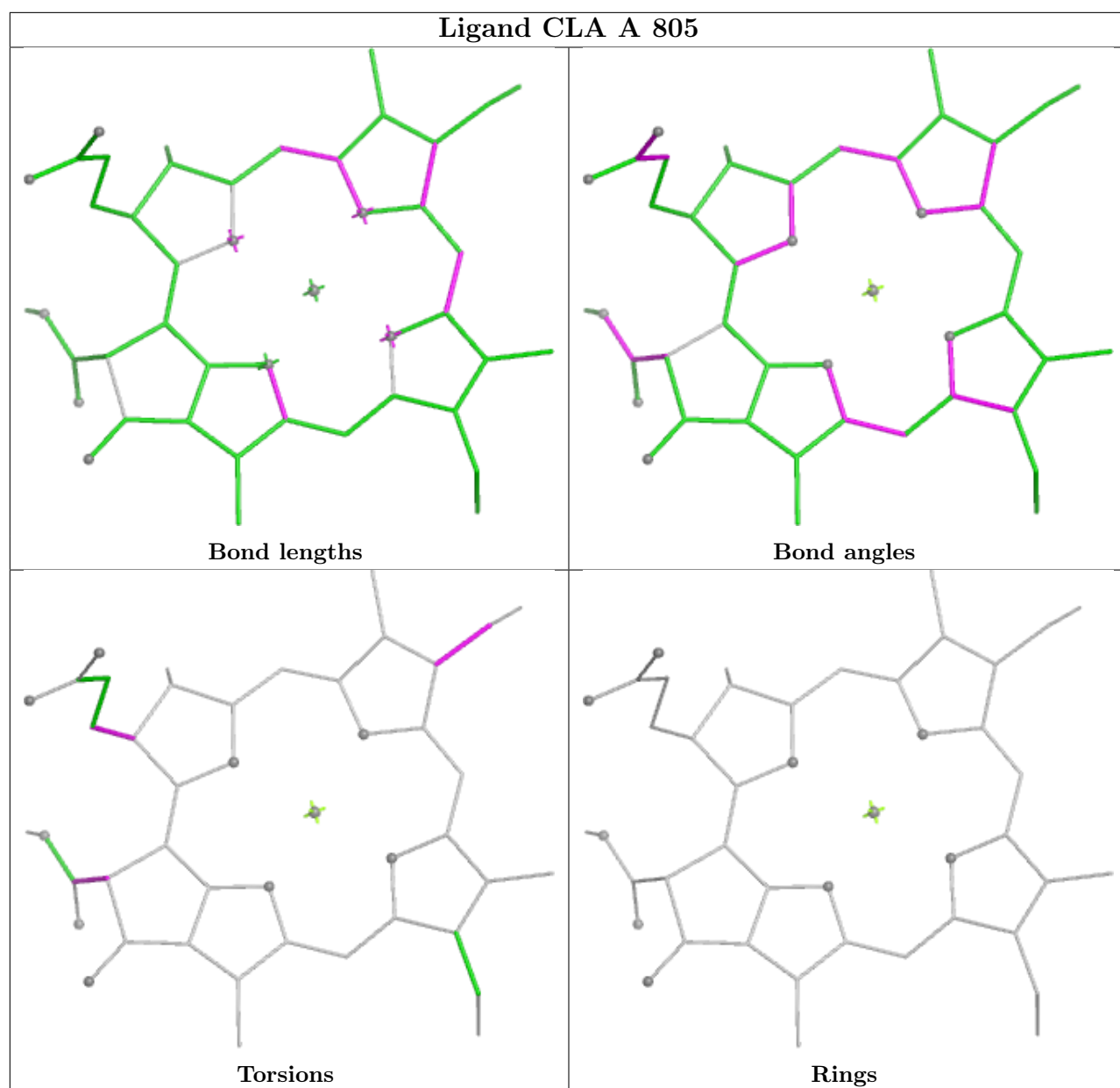


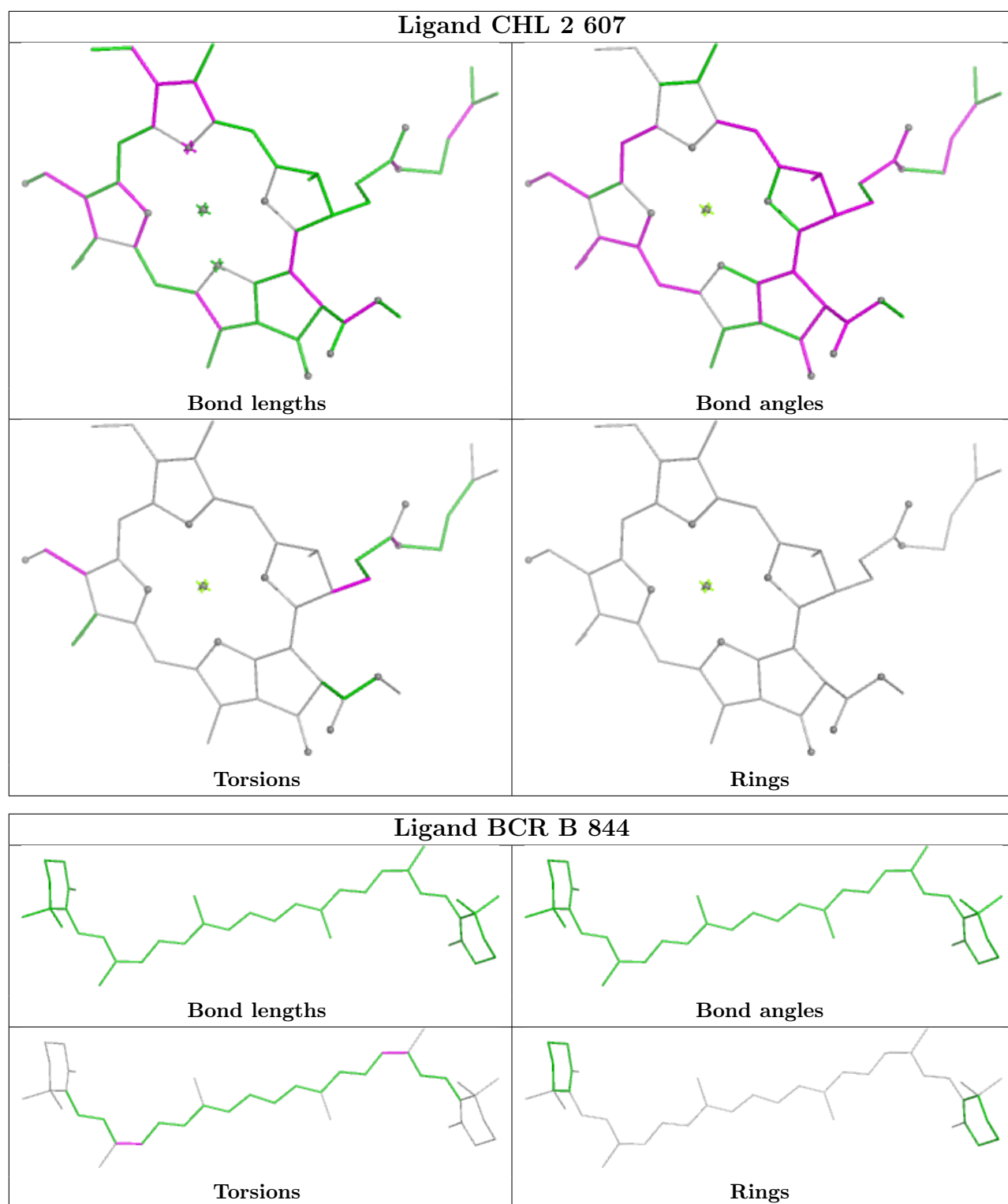
Ligand CHL 3 616

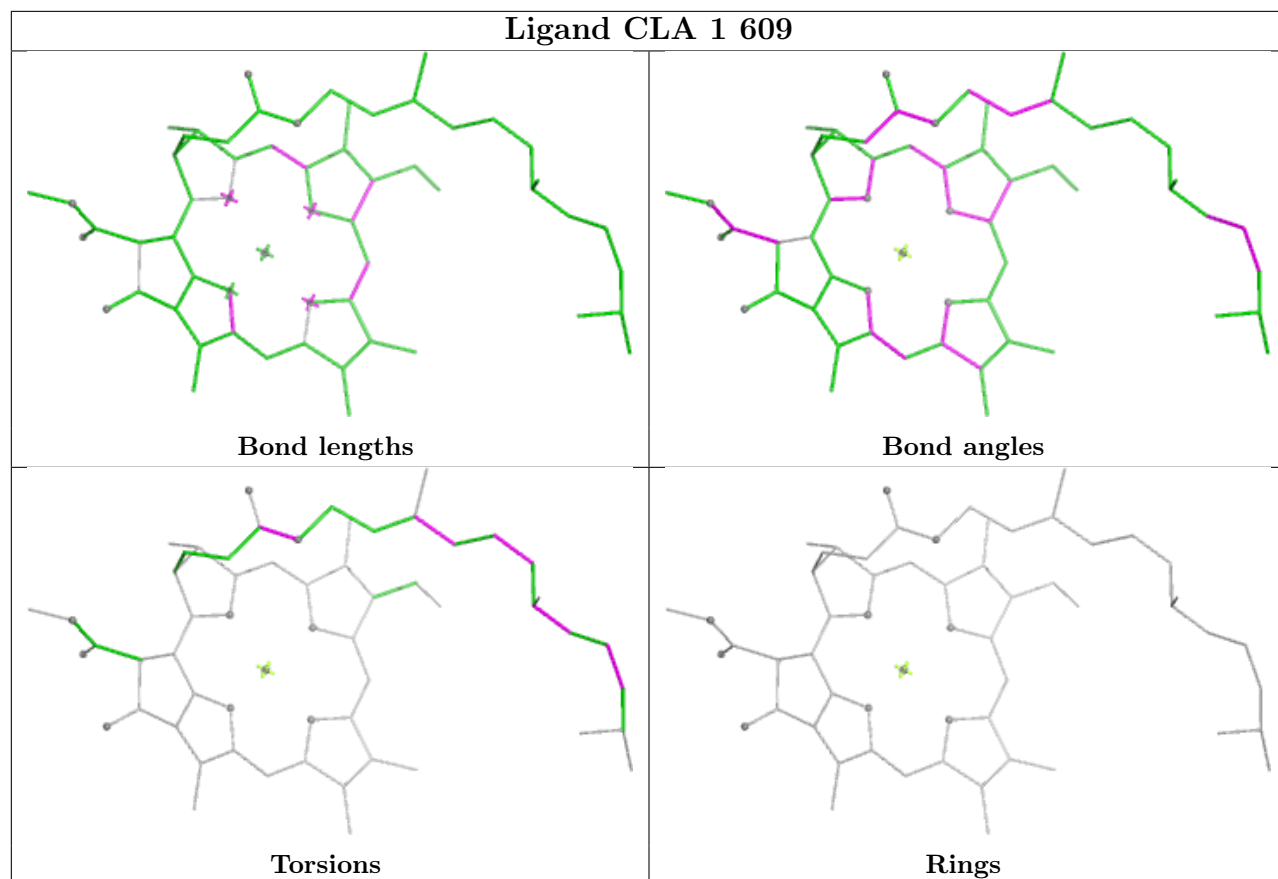


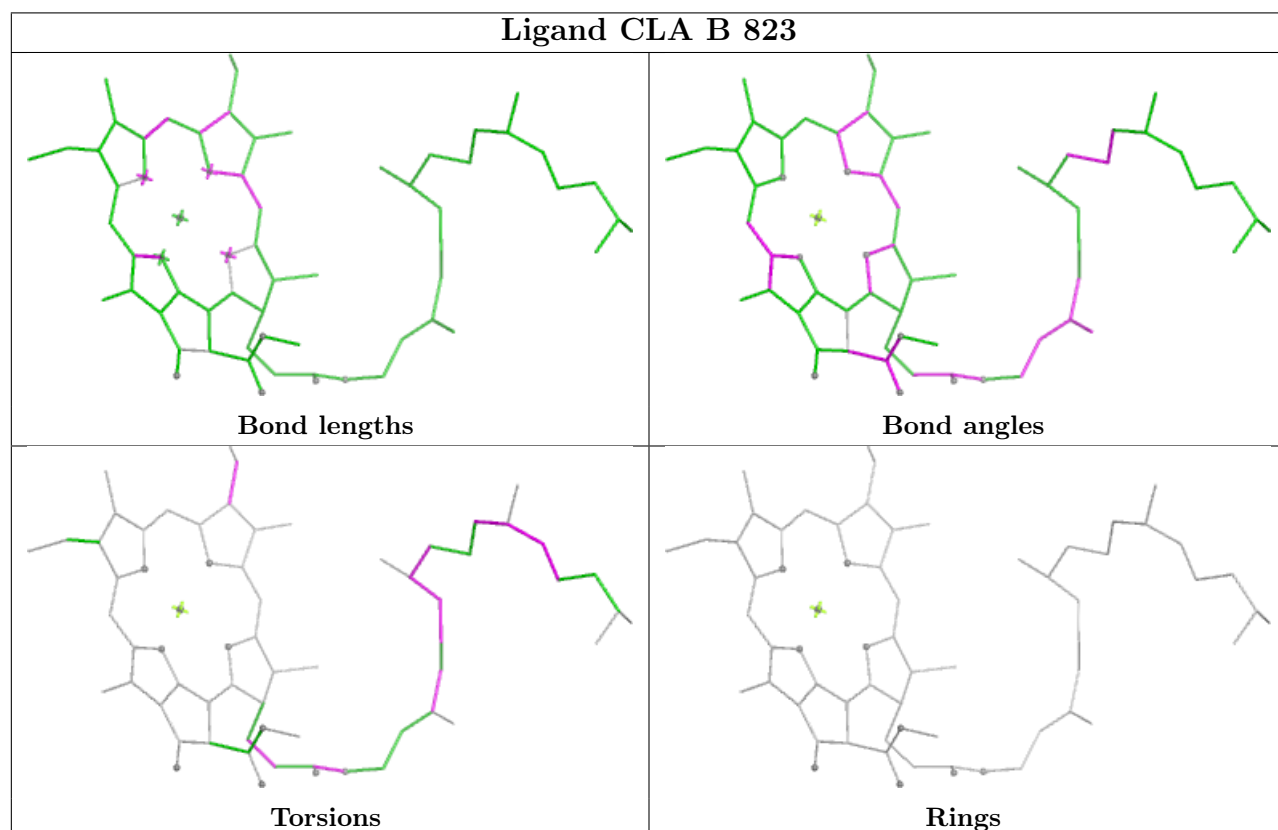
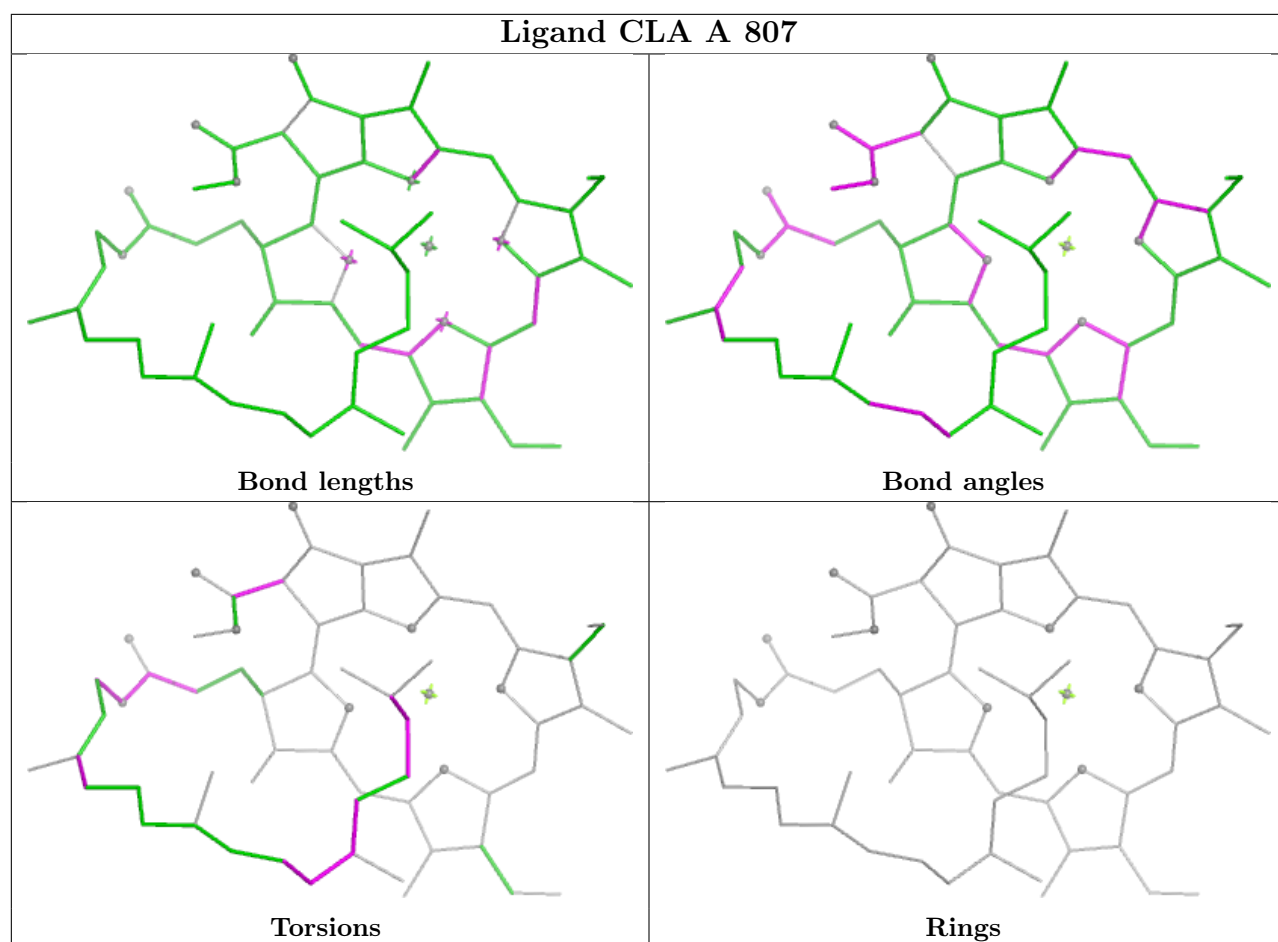
Ligand CLA B 815



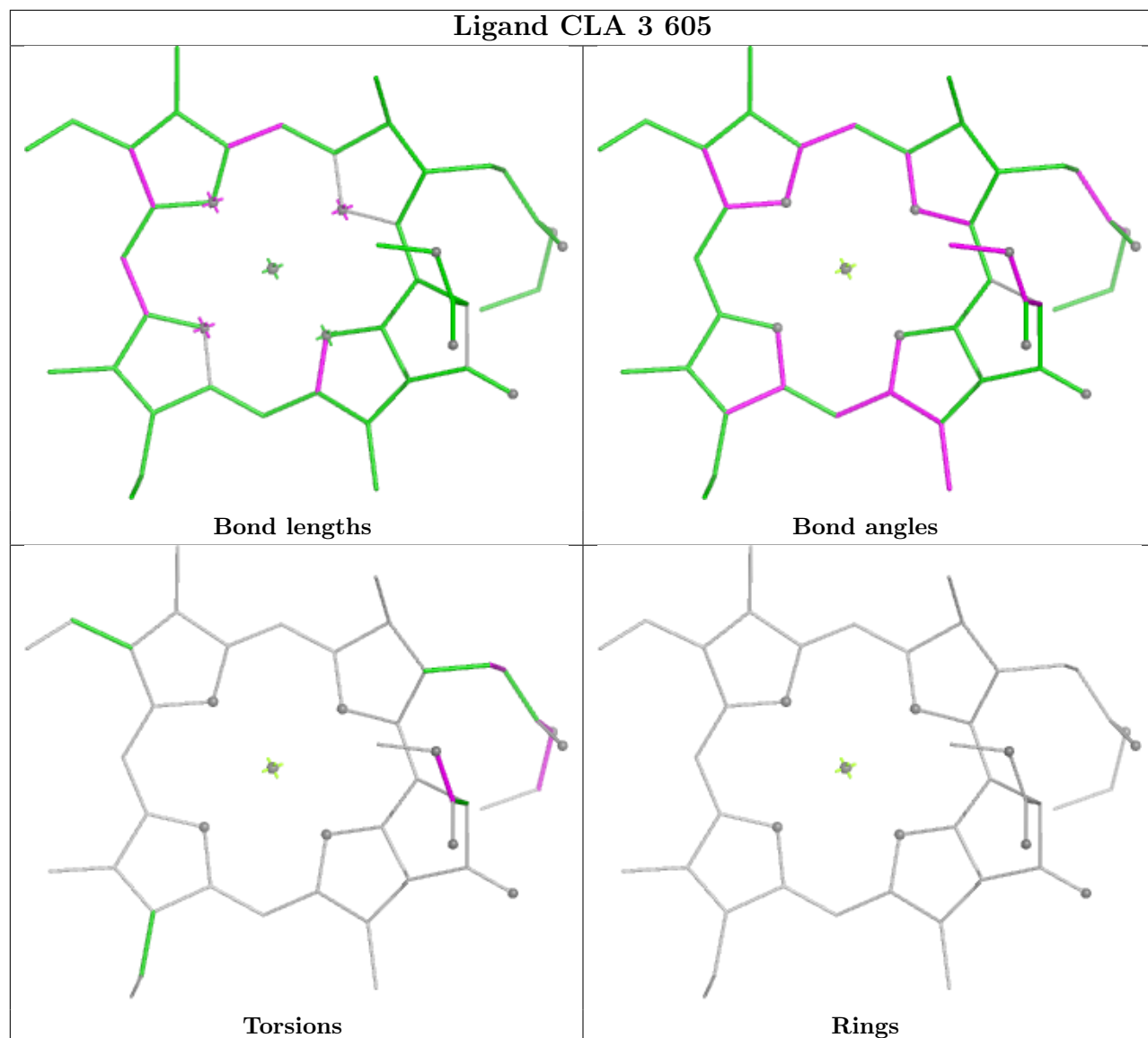




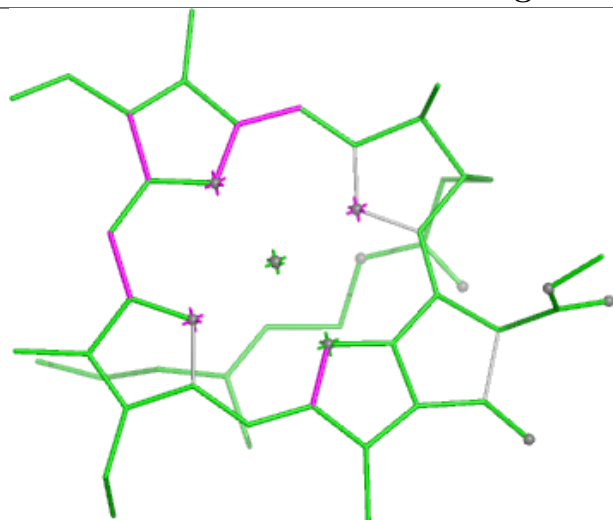




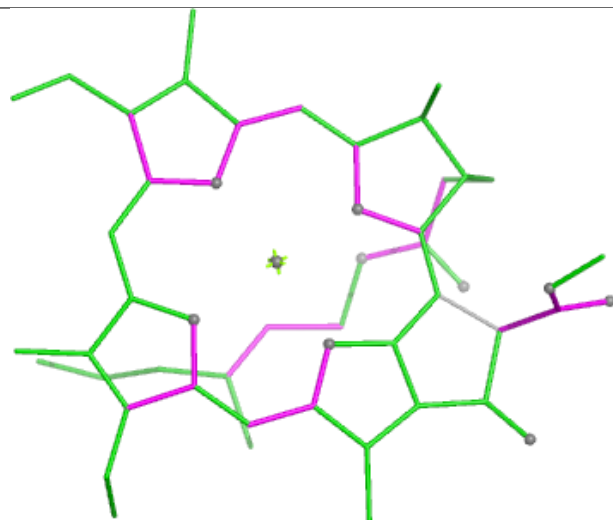
Ligand CLA 3 605



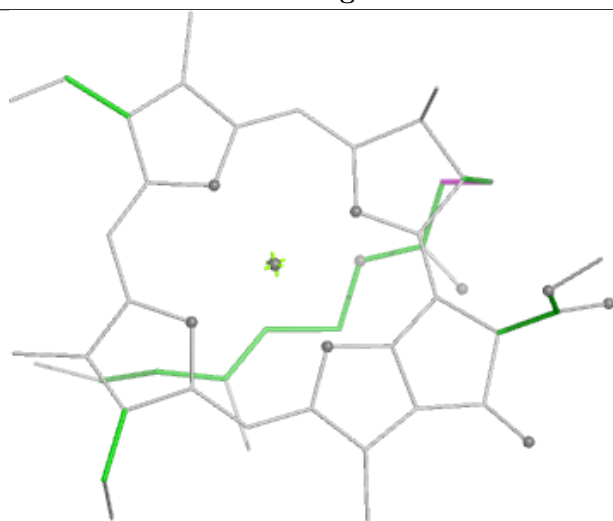
Ligand CLA B 806



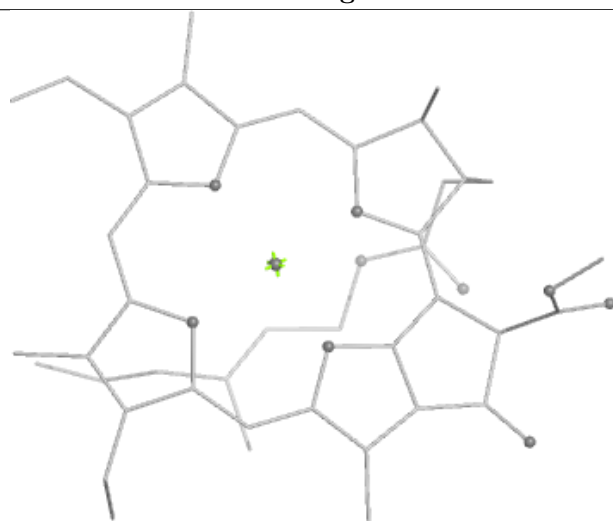
Bond lengths



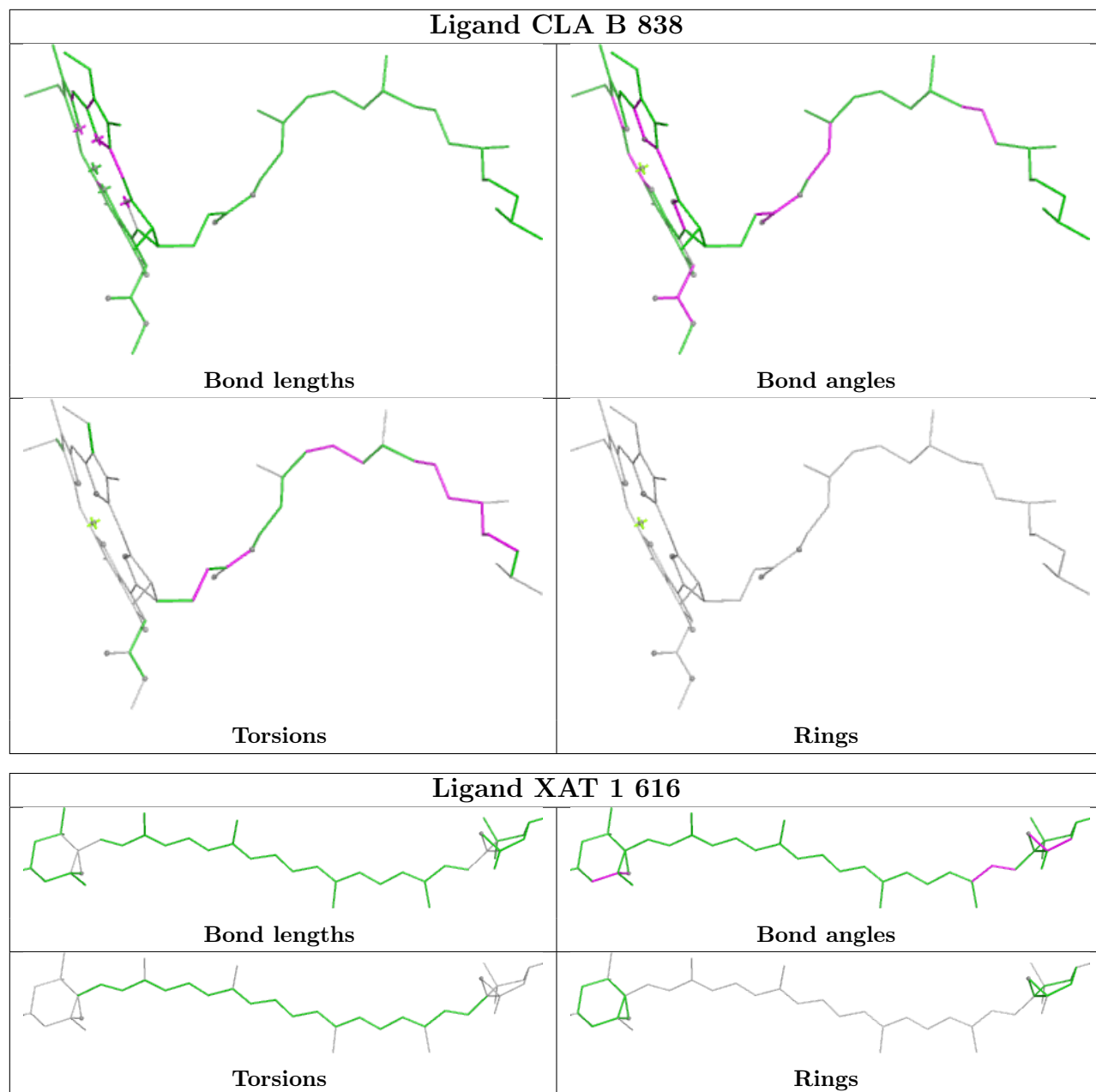
Bond angles



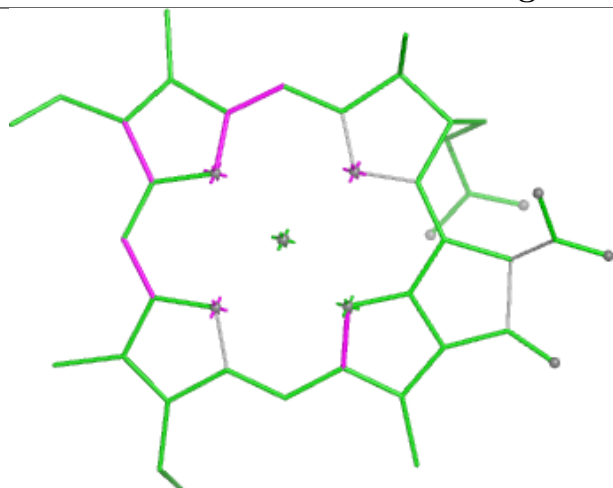
Torsions



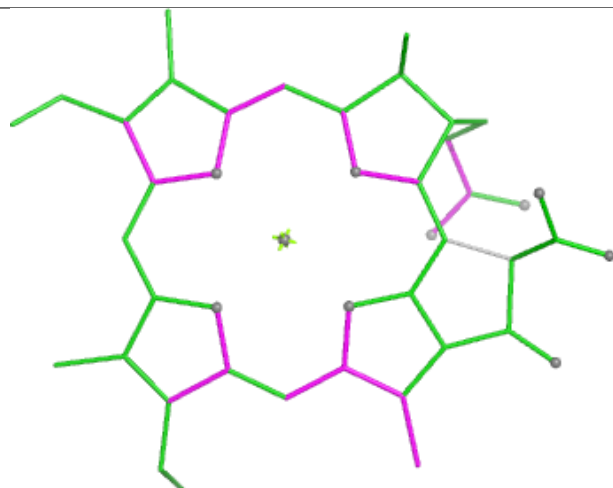
Rings



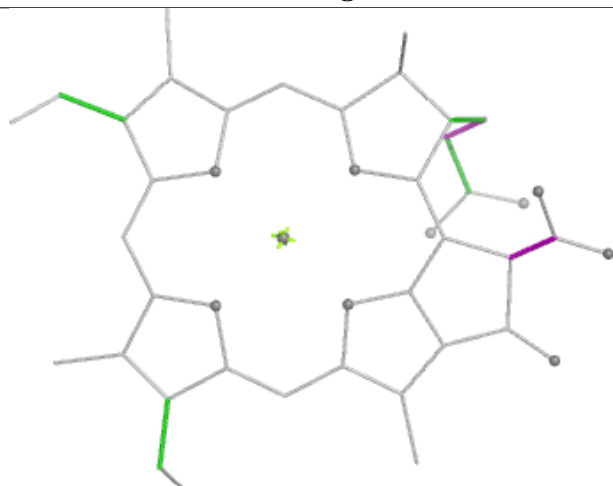
Ligand CLA 3 611



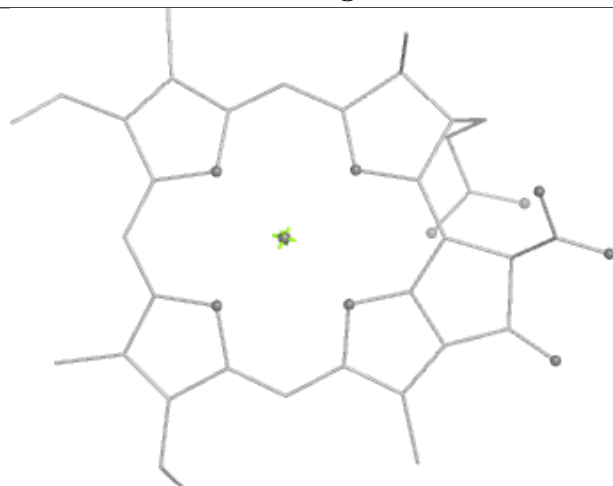
Bond lengths



Bond angles

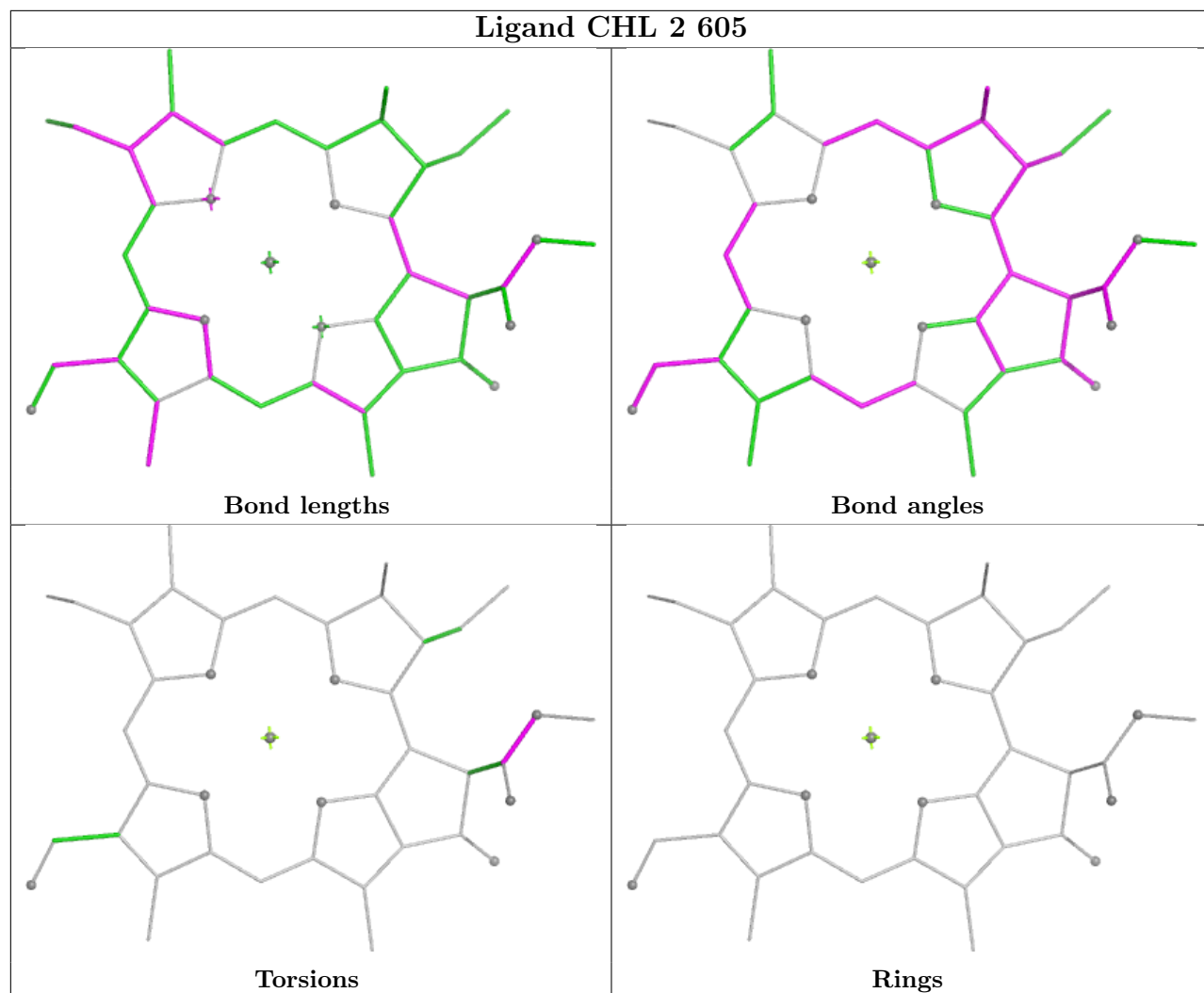


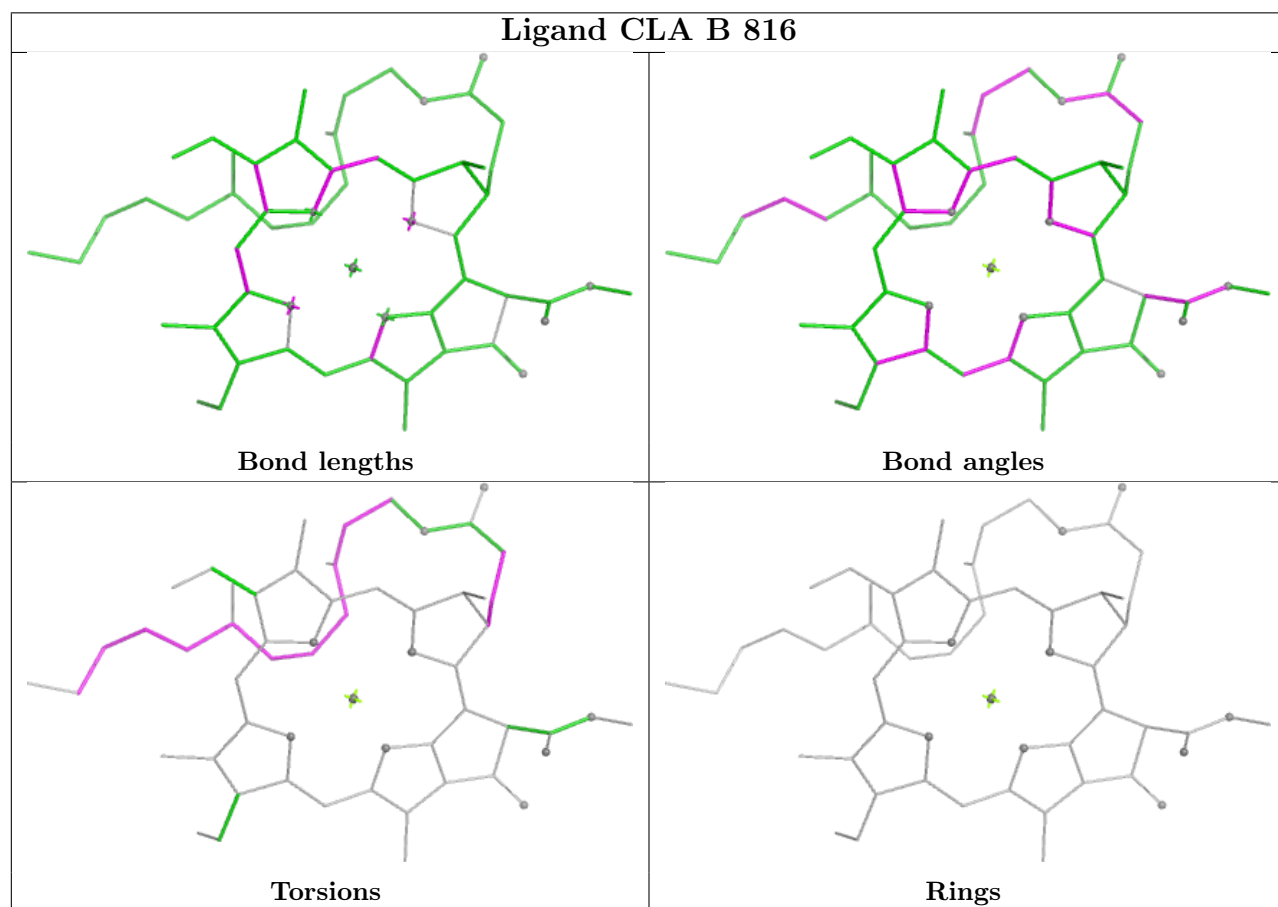
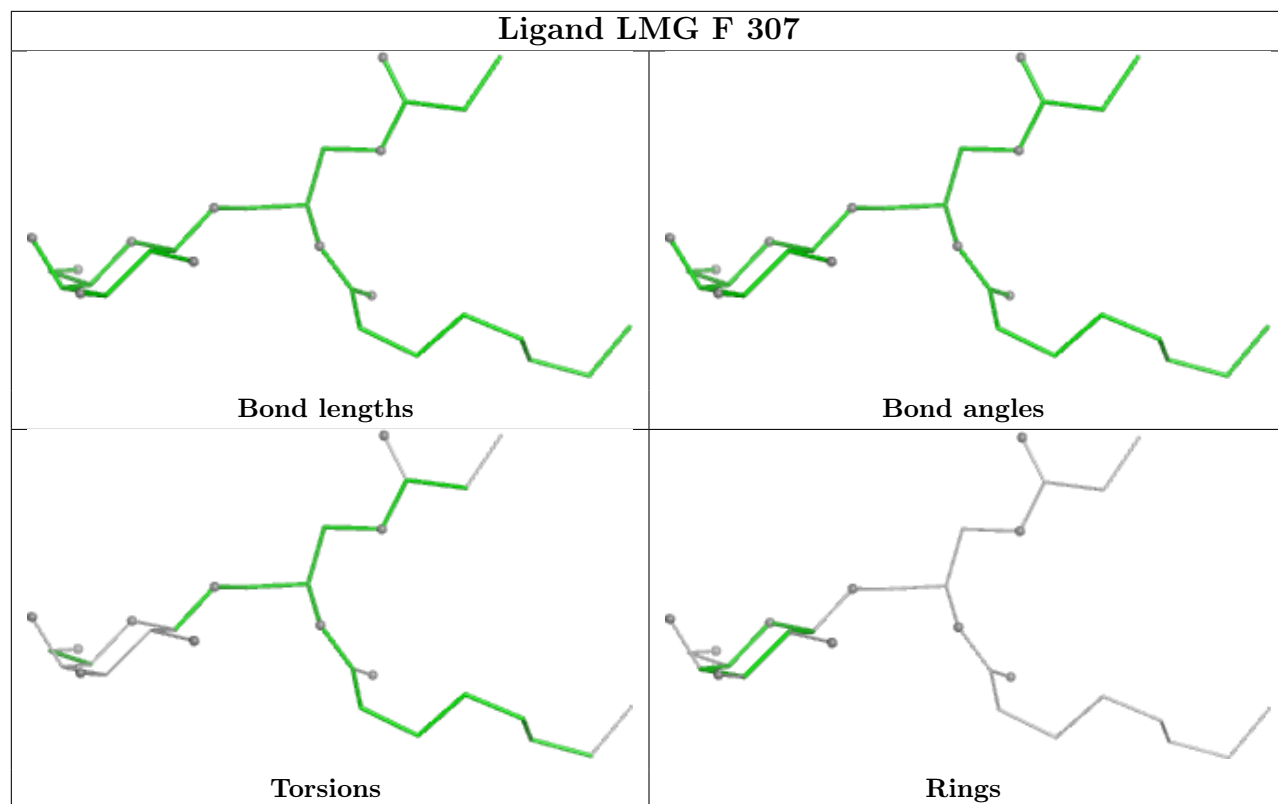
Torsions

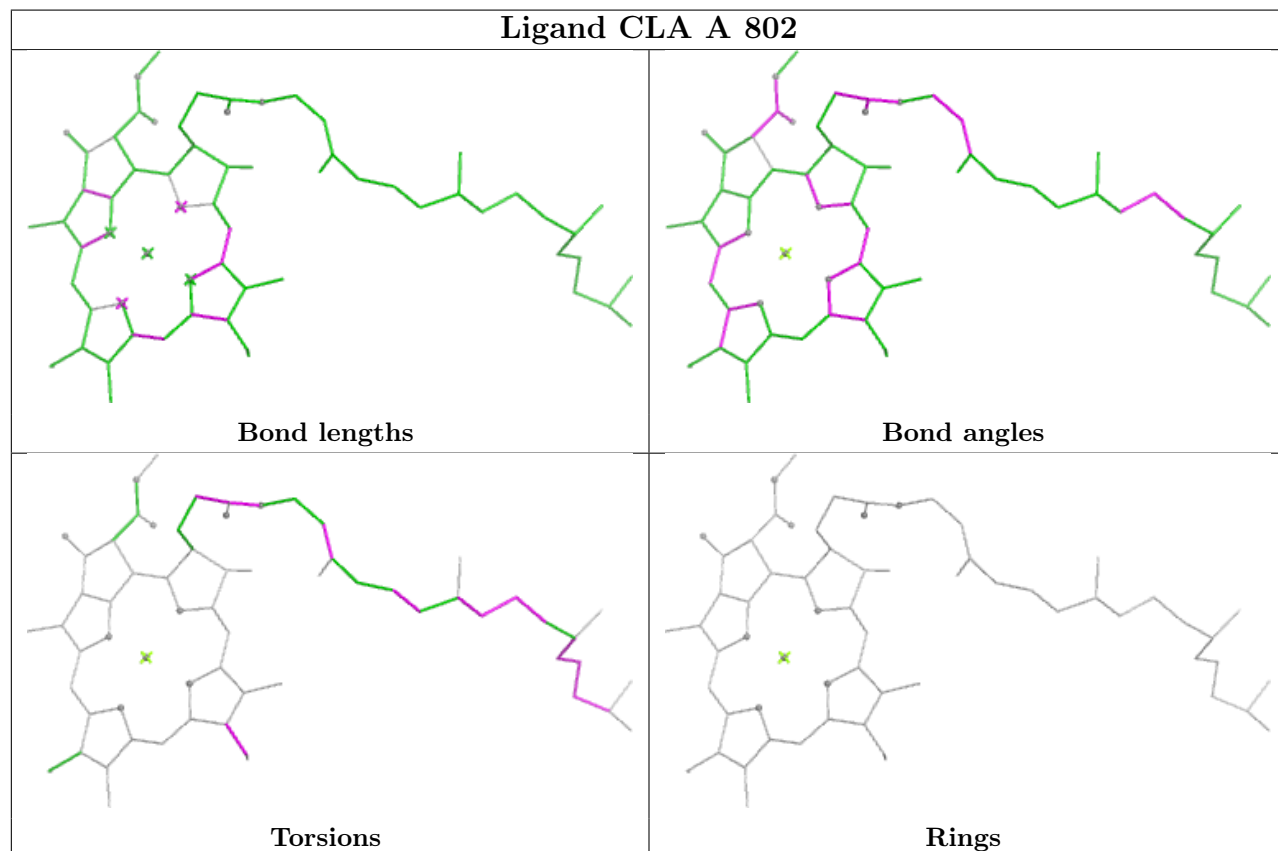
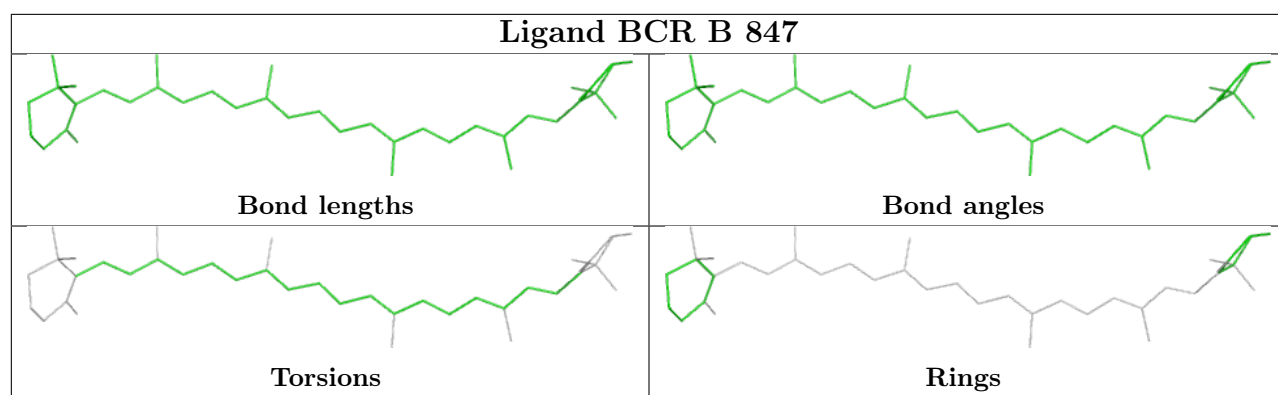


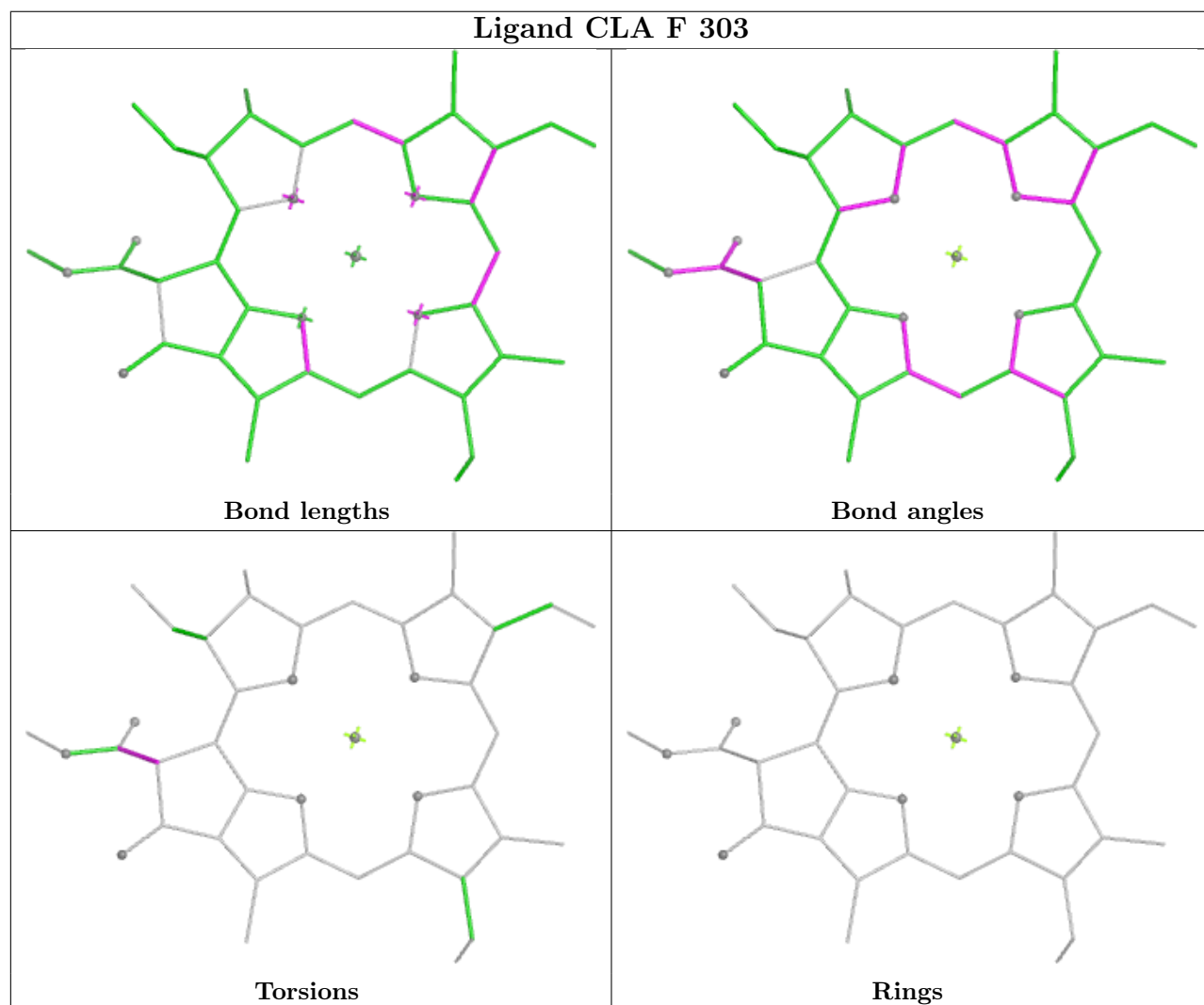
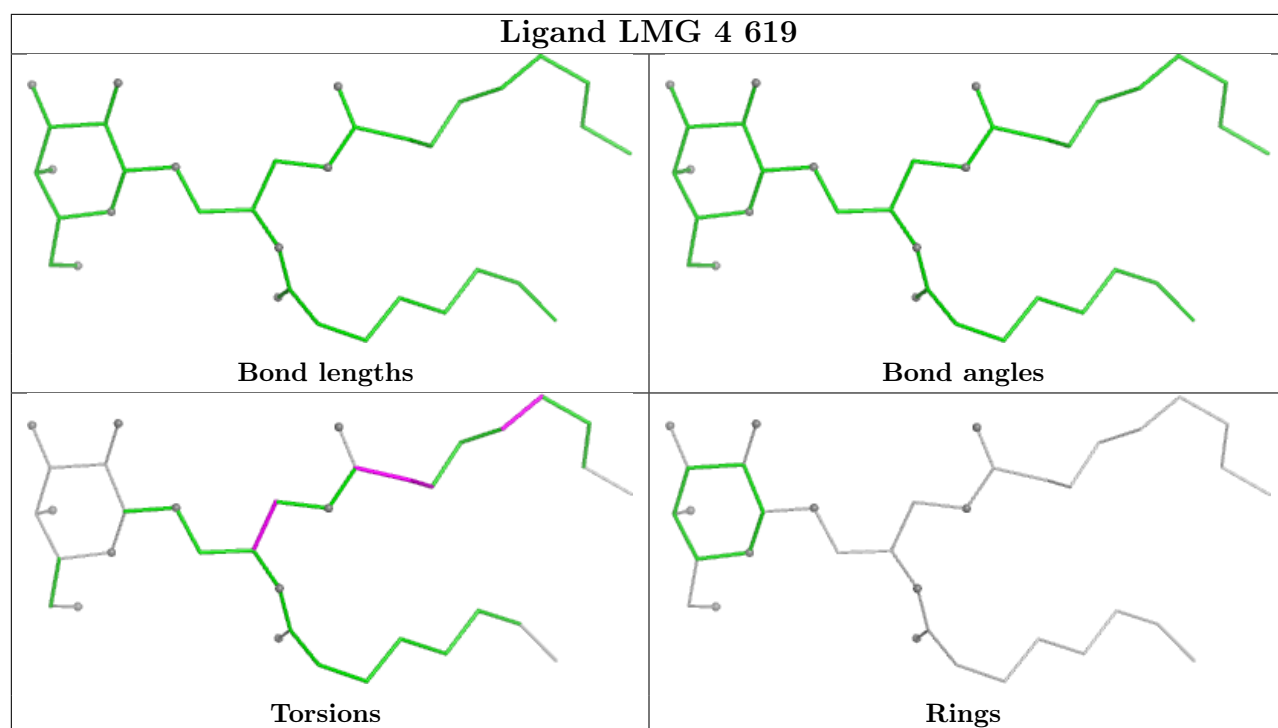
Rings

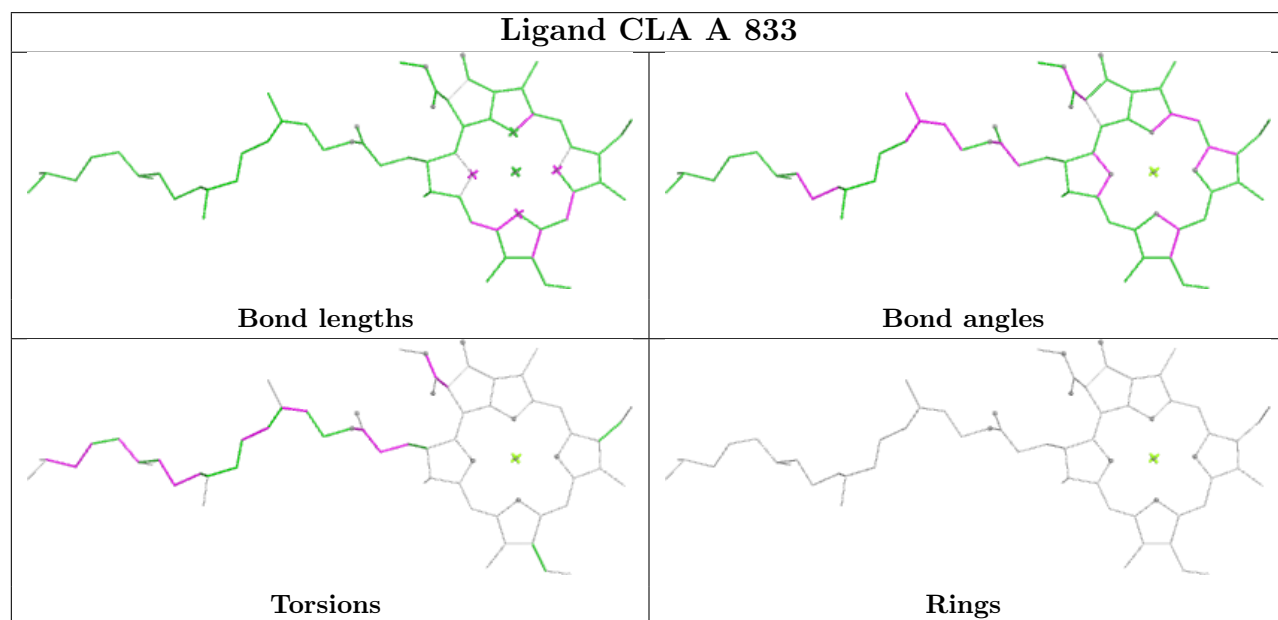
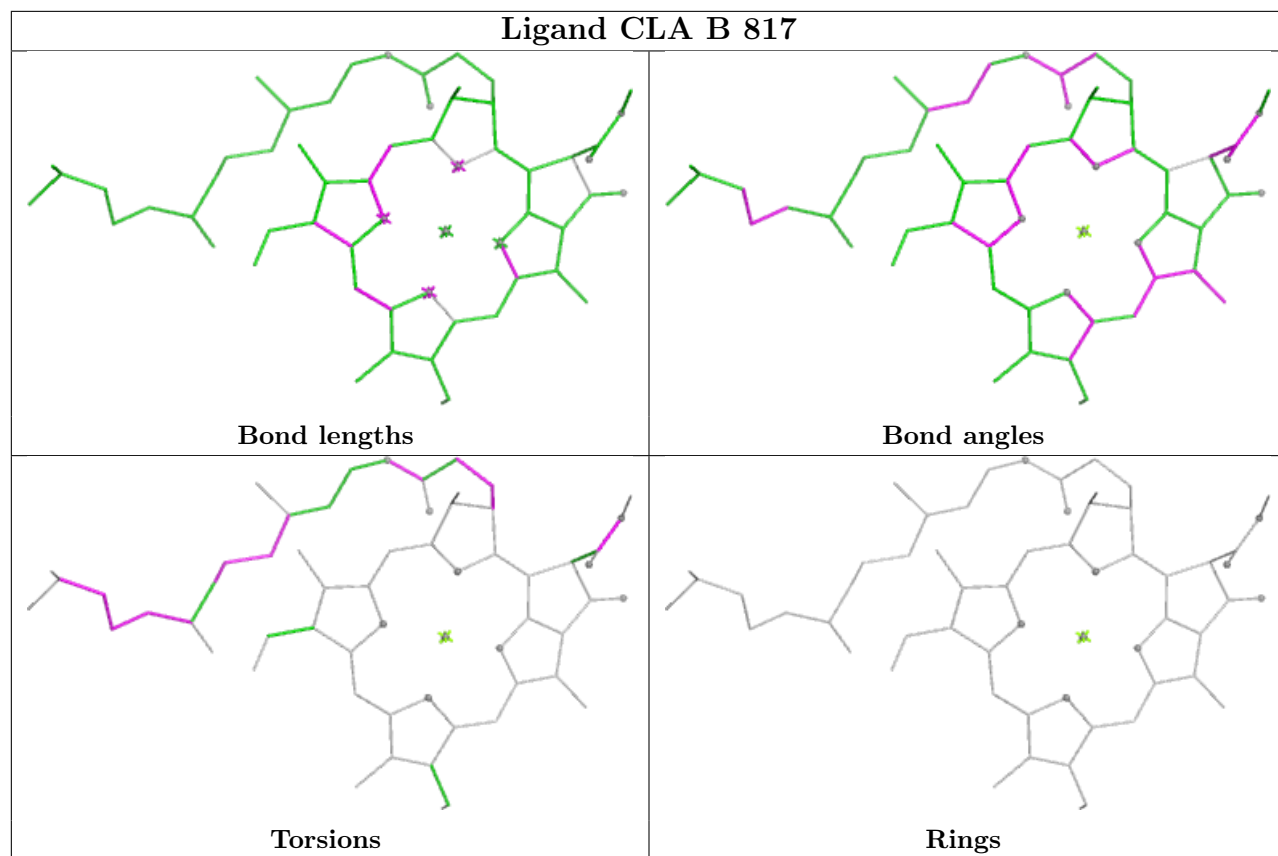
Ligand CHL 2 605



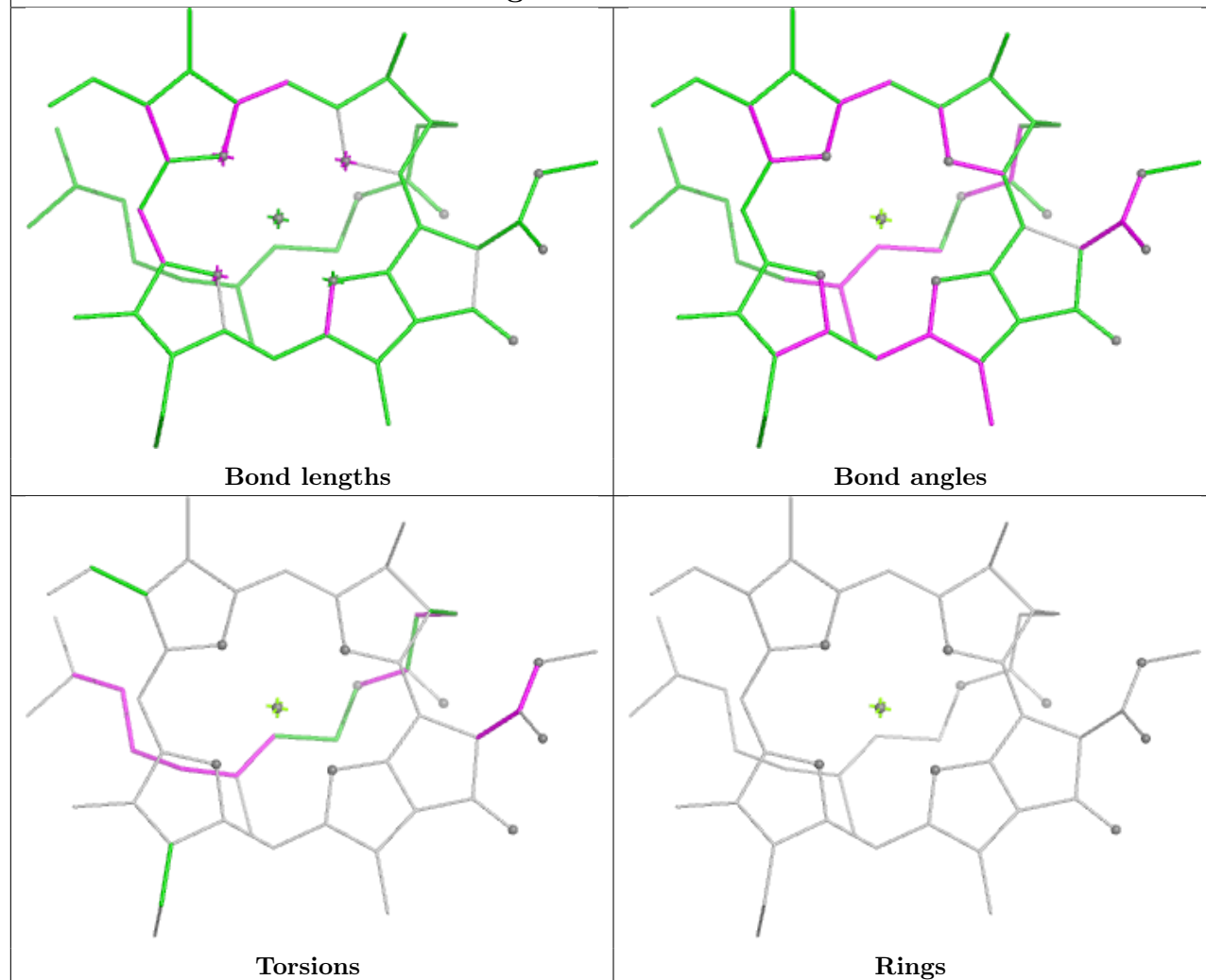




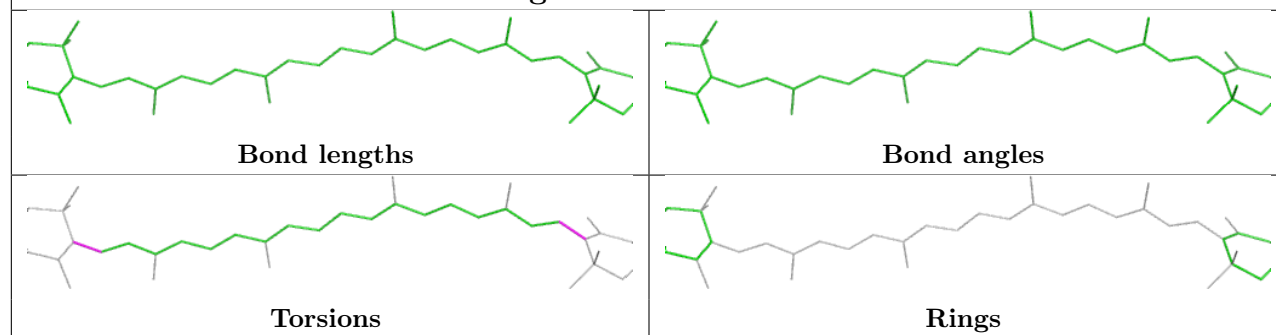


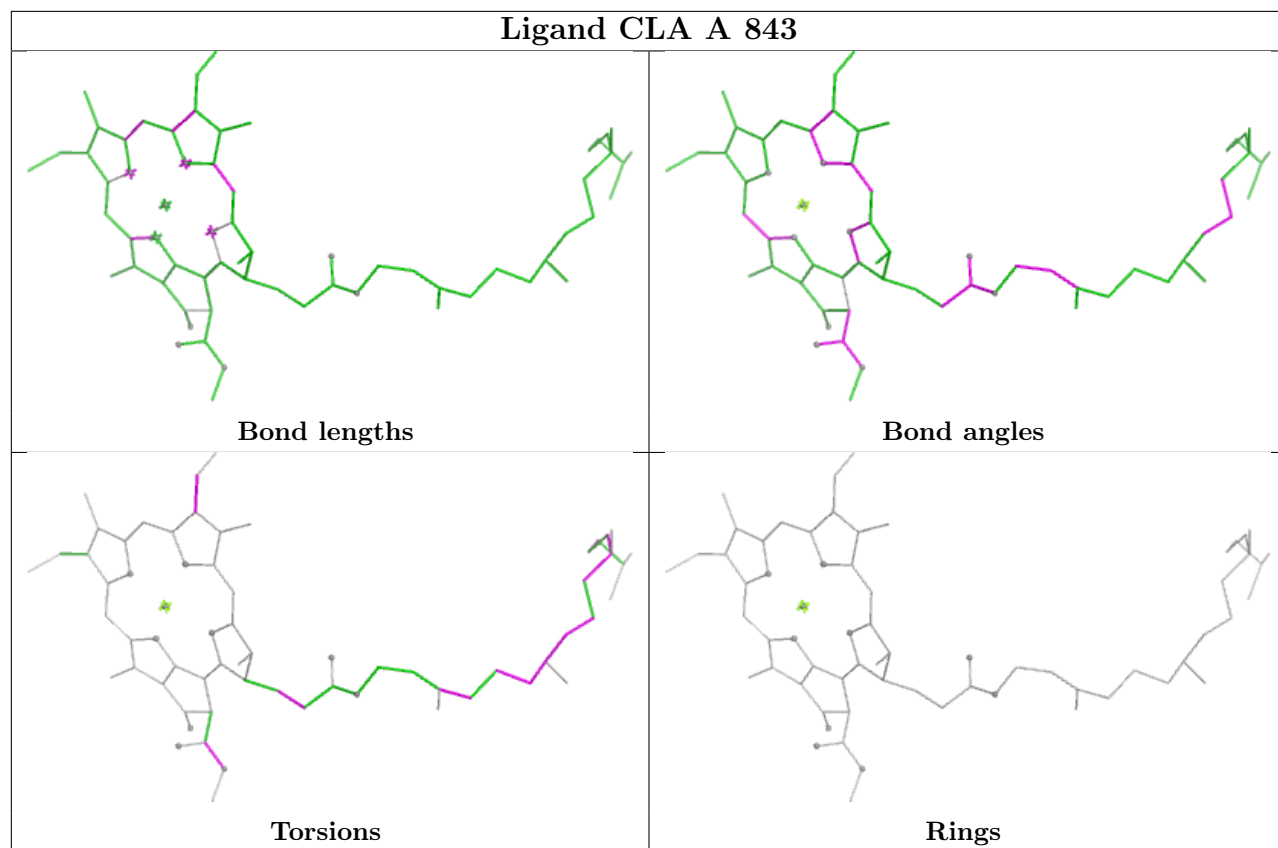


Ligand CLA 2 612

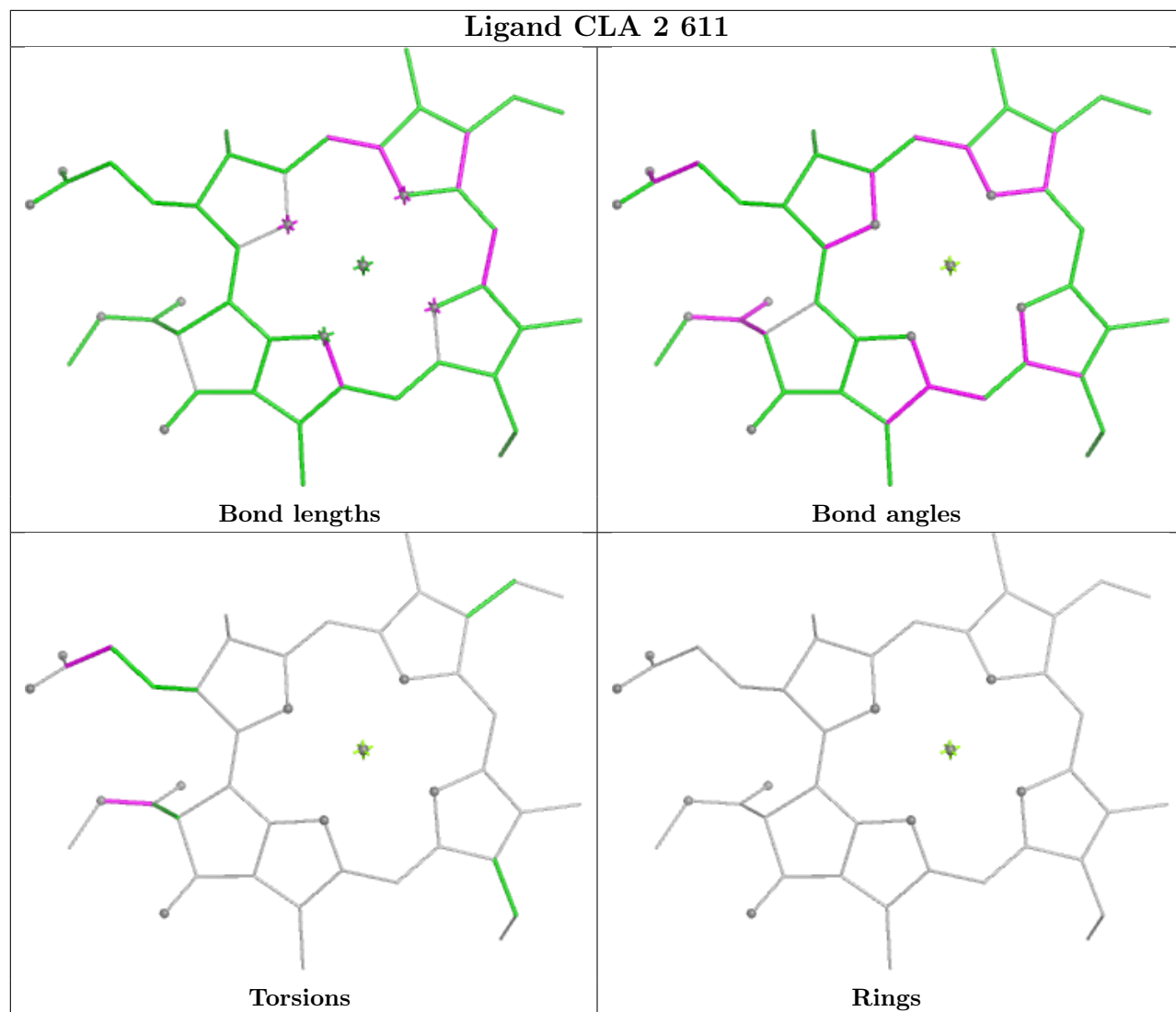


Ligand BCR K 205

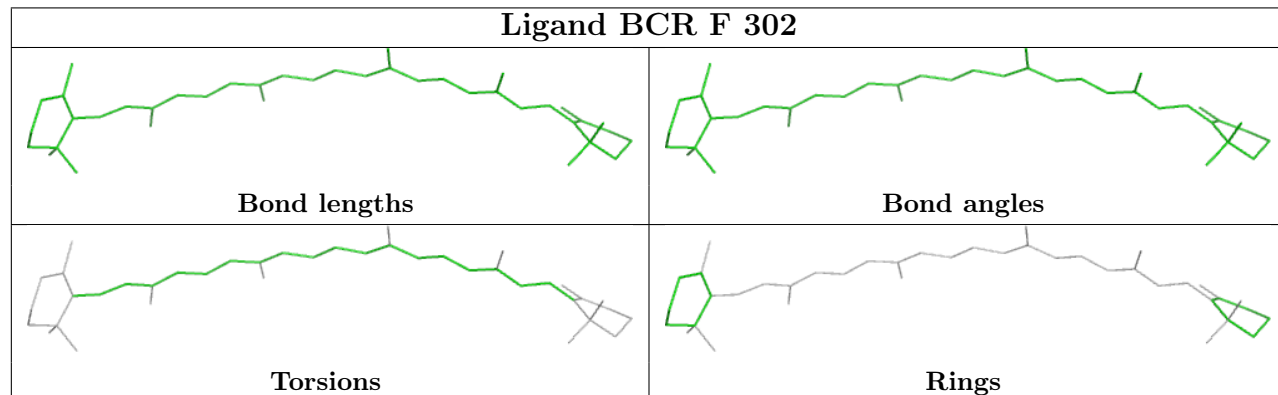


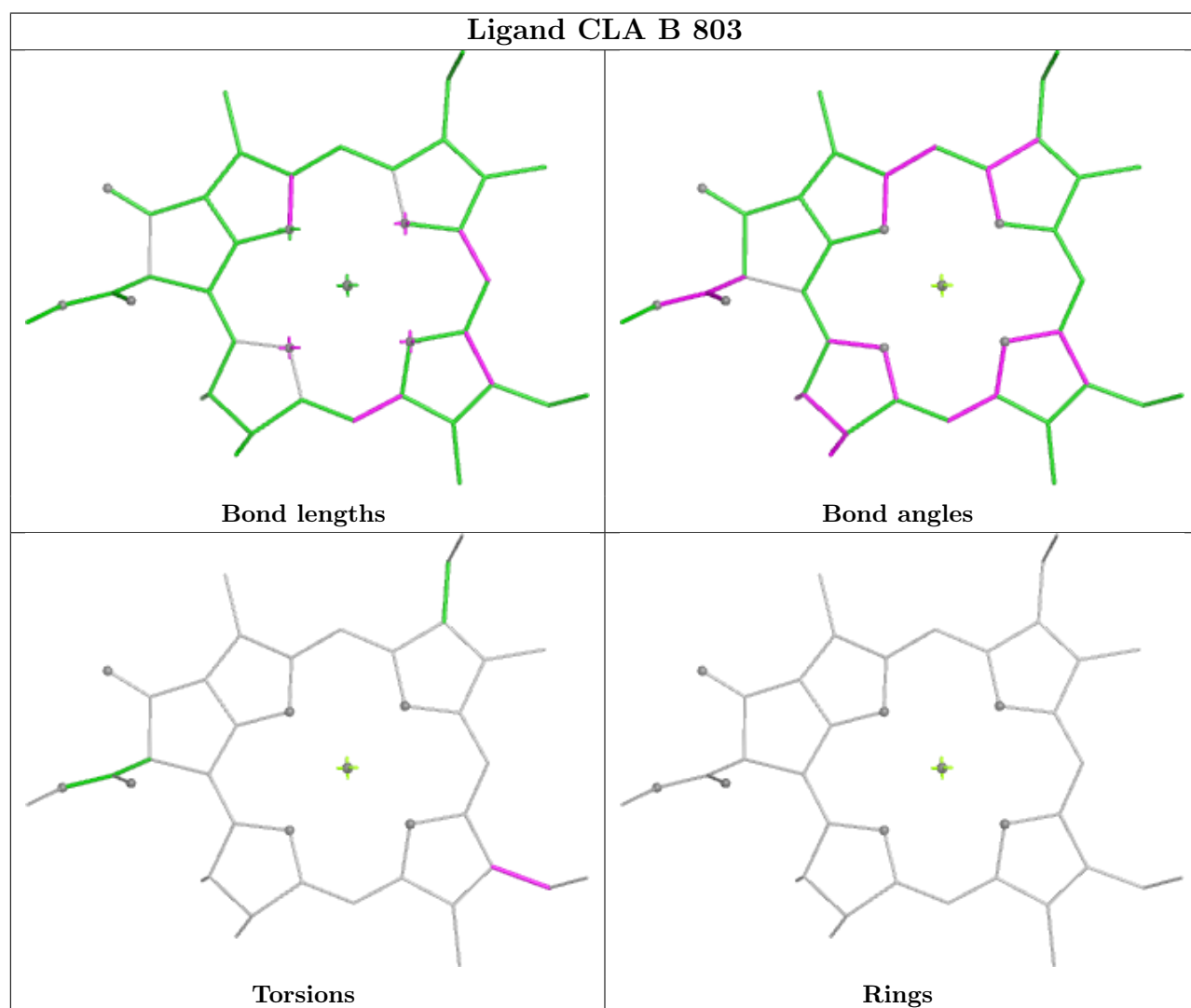
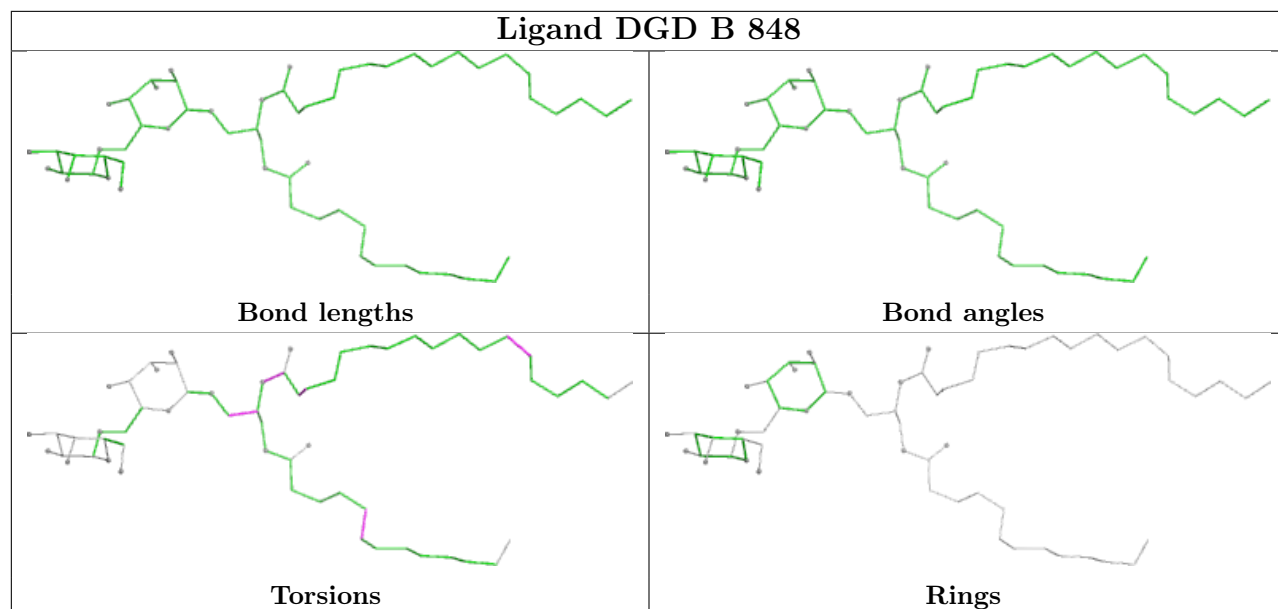


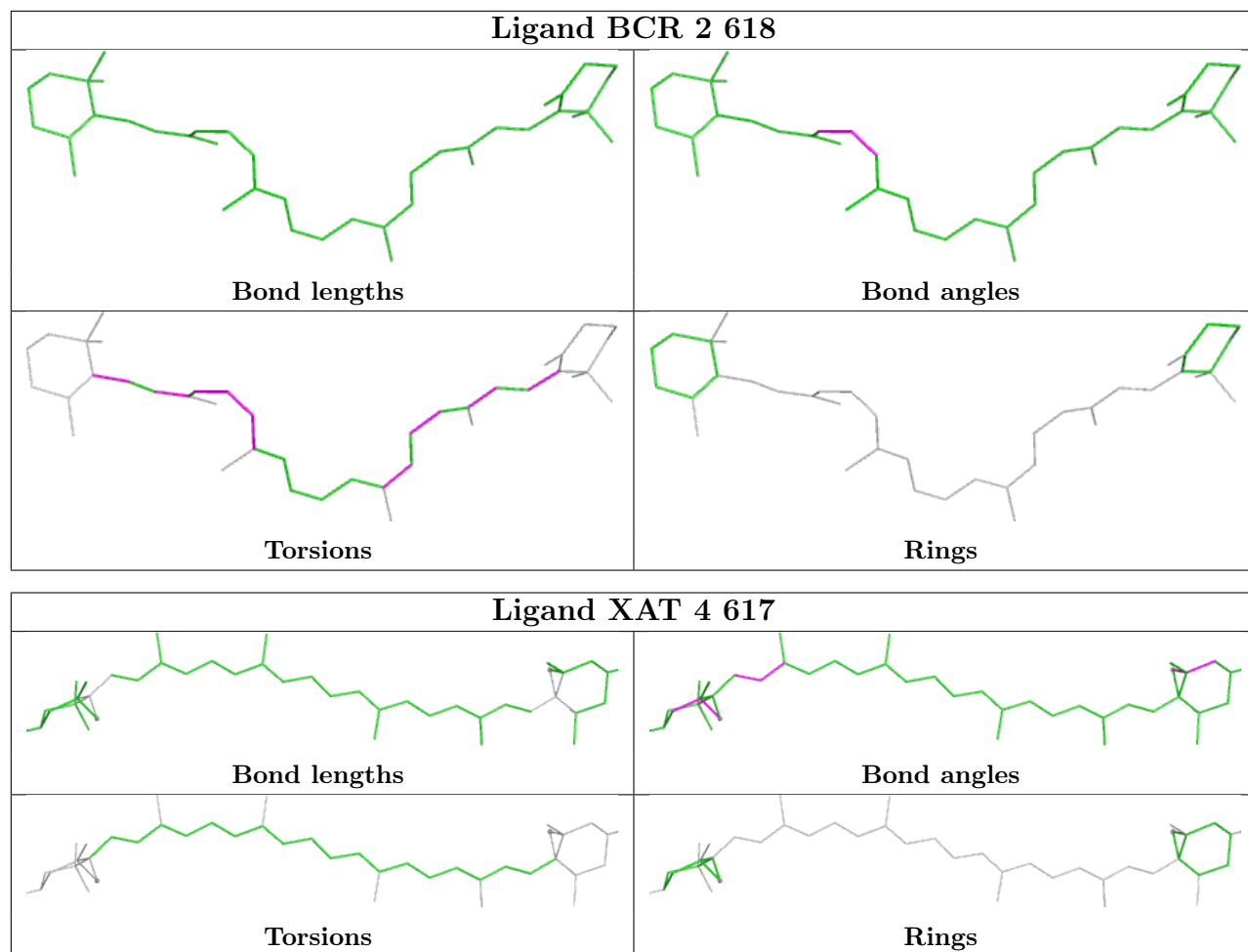
Ligand CLA 2 611

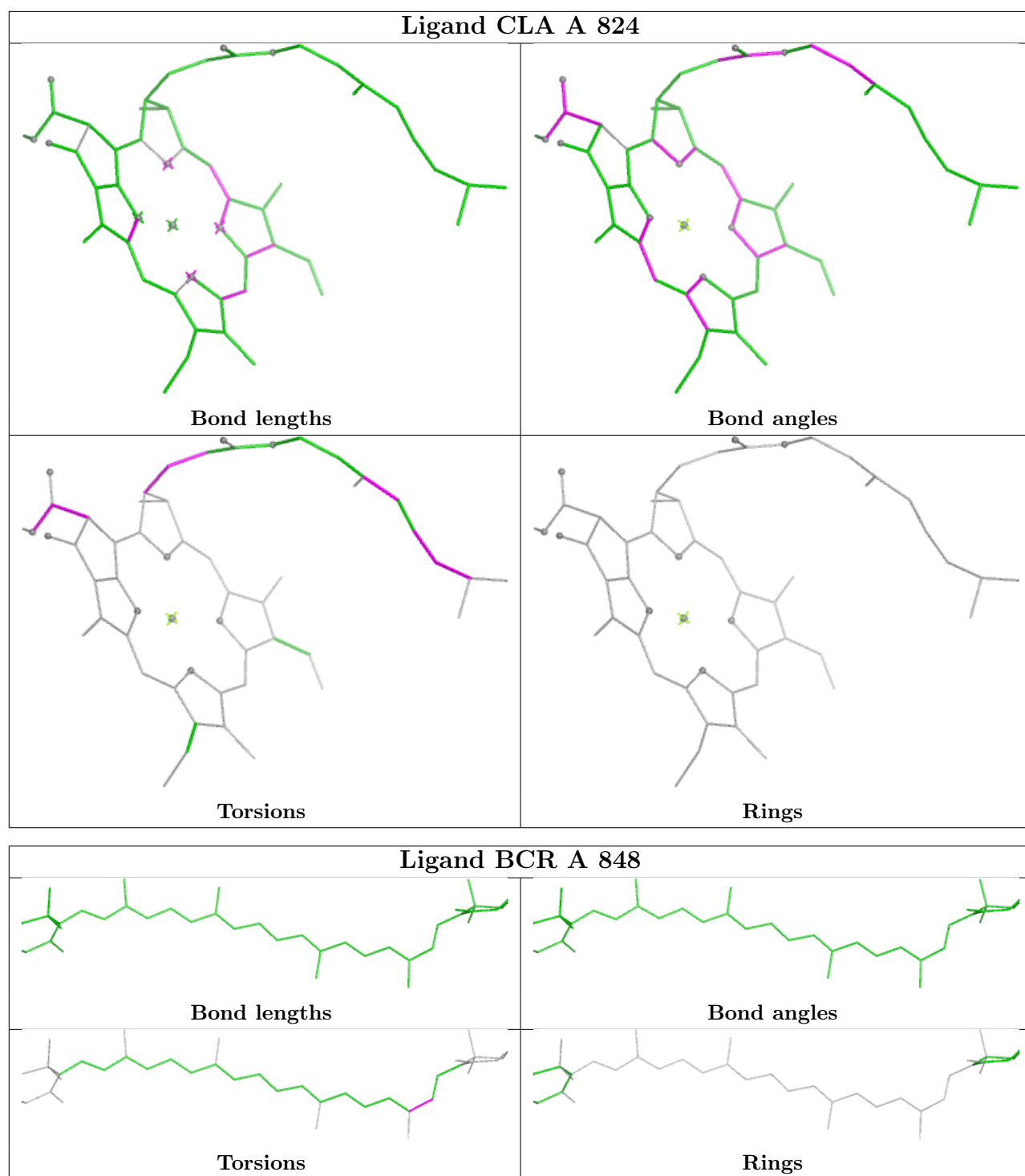


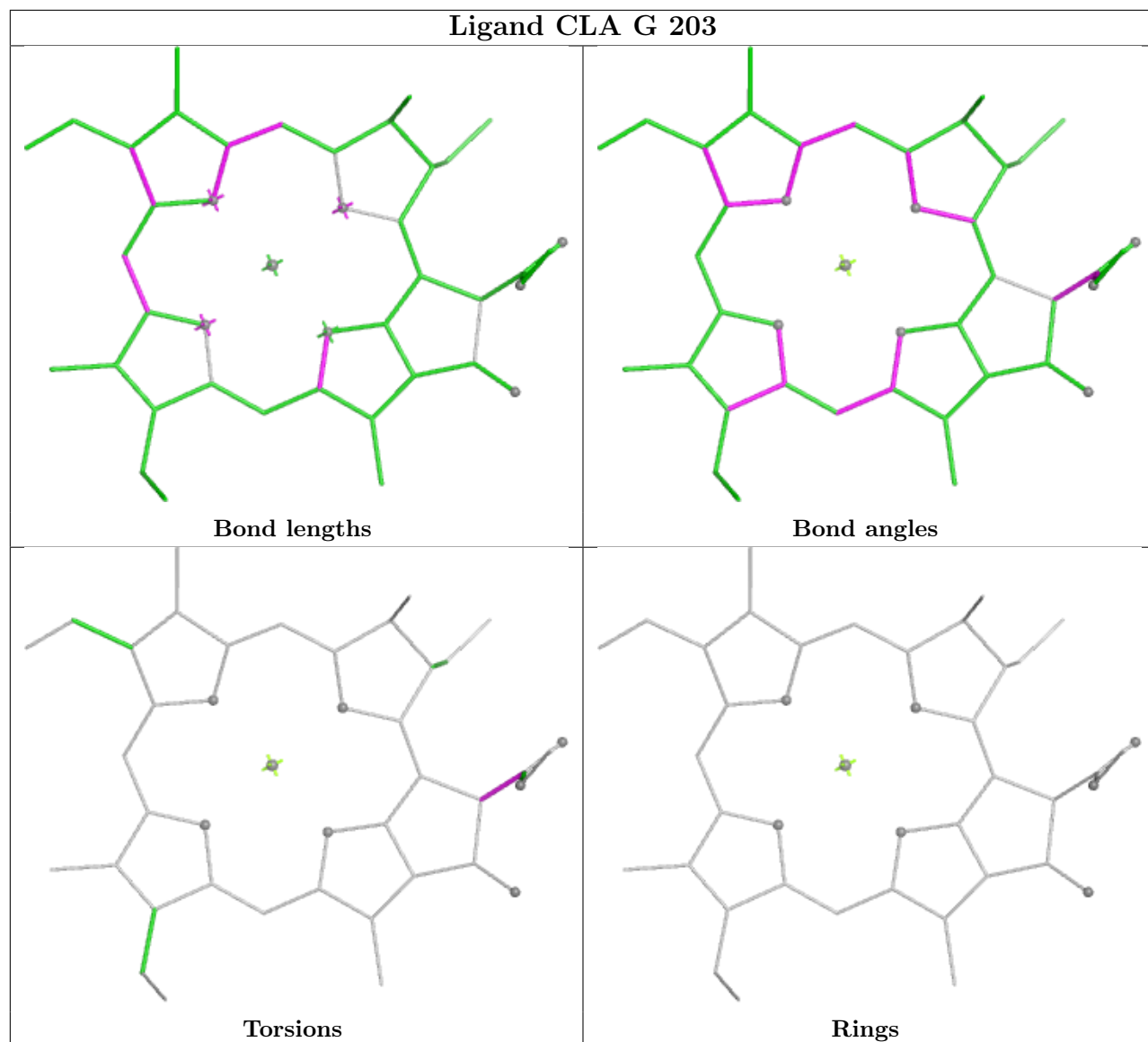
Ligand BCR F 302



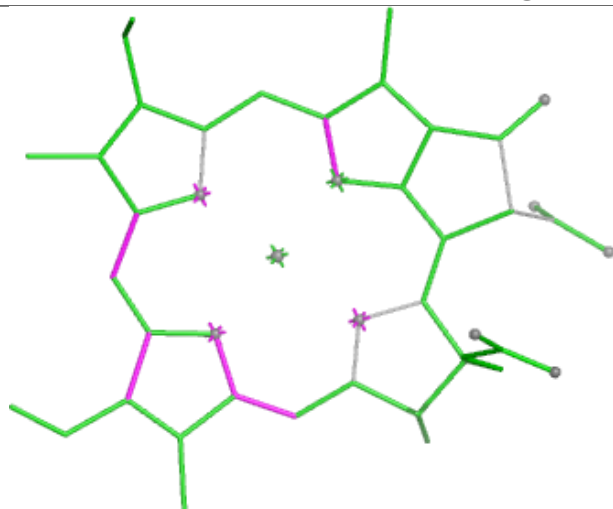




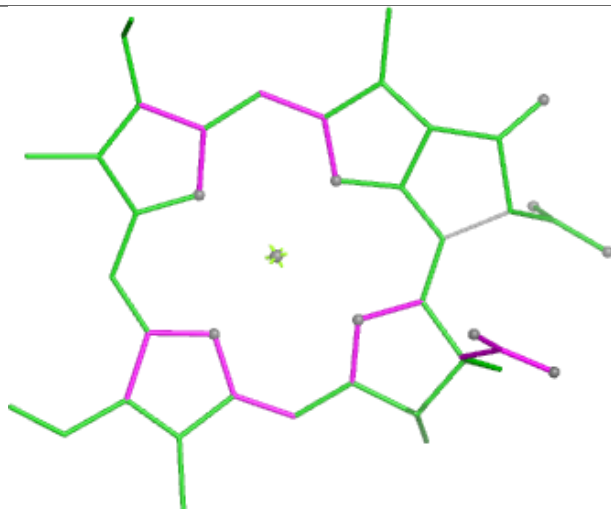




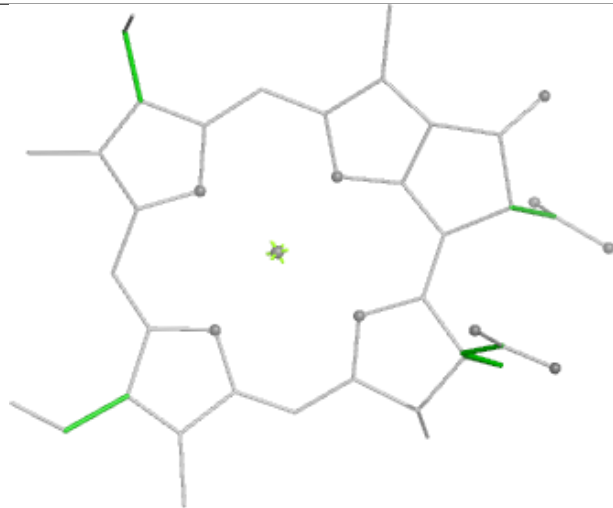
Ligand CLA 1 607



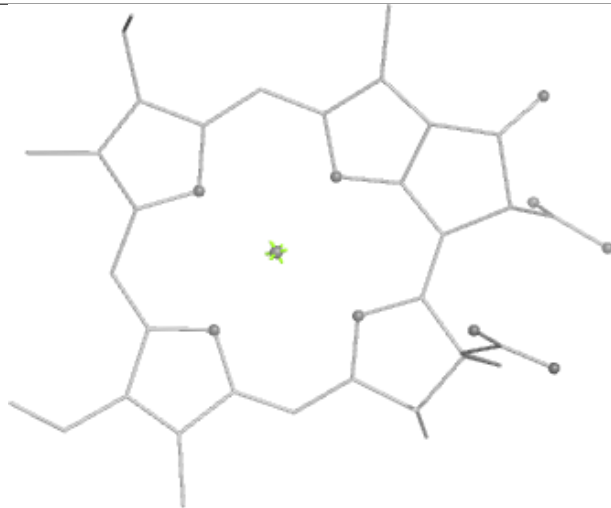
Bond lengths



Bond angles

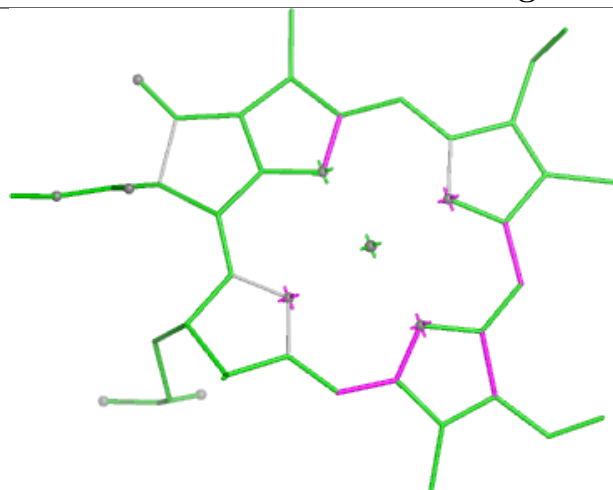


Torsions

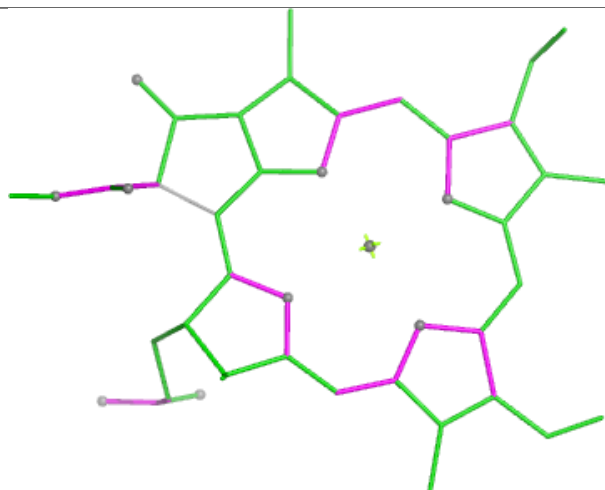


Rings

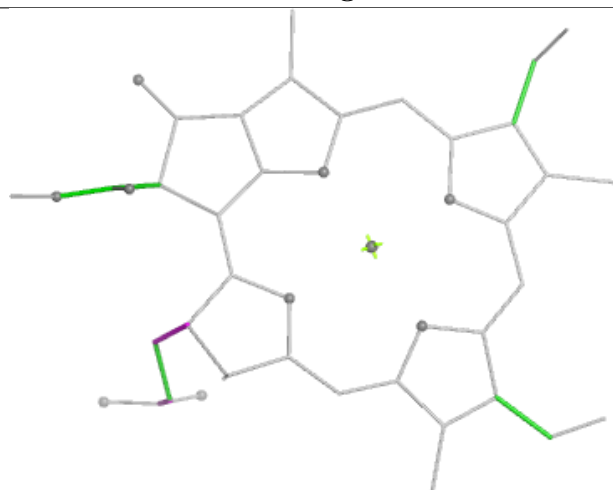
Ligand CLA 2 608



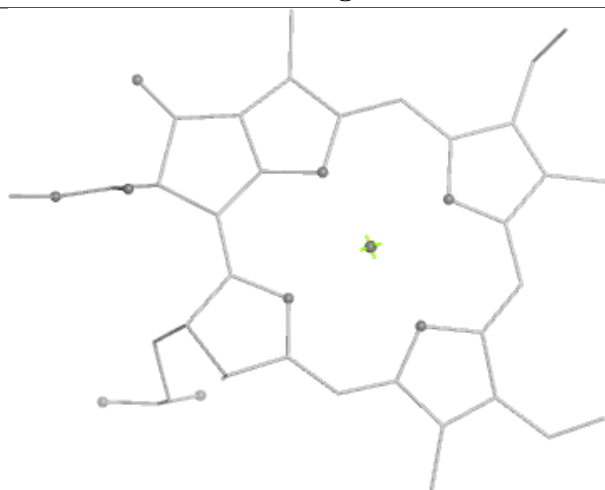
Bond lengths



Bond angles



Torsions



Rings

Ligand BCR L 301



Bond lengths



Bond angles

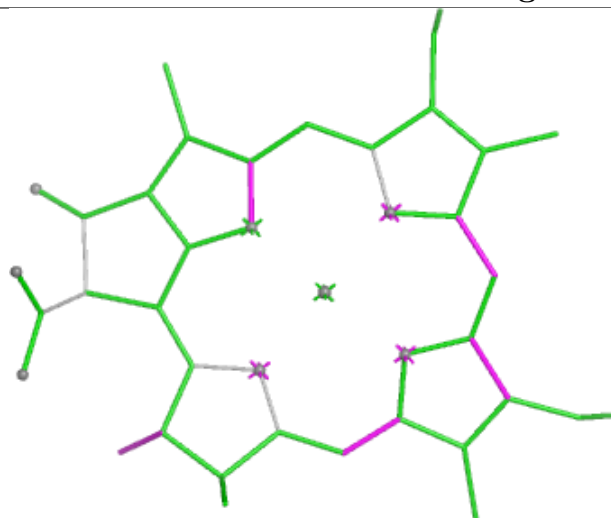


Torsions

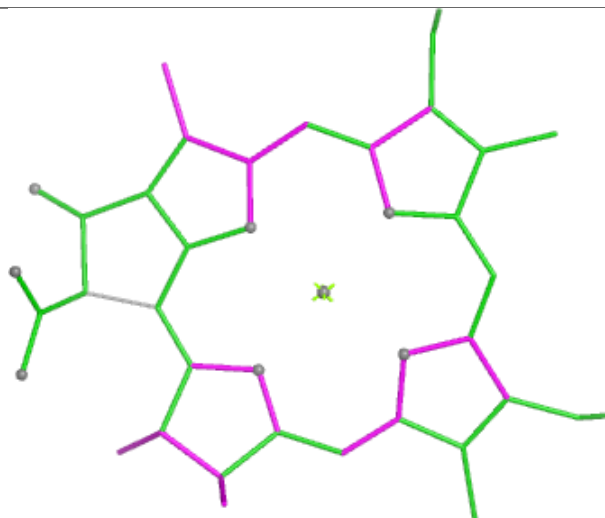


Rings

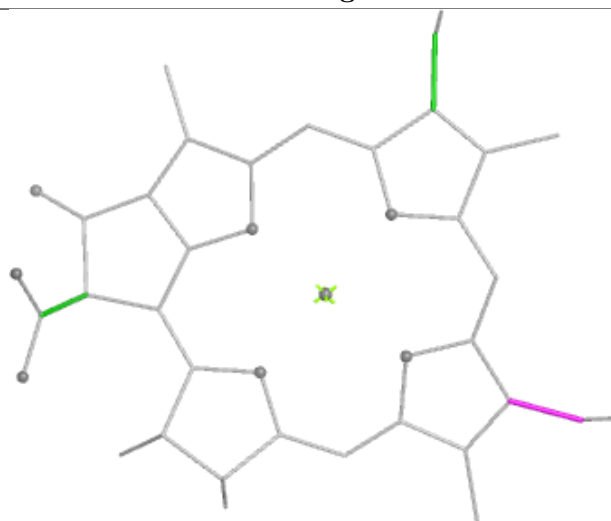
Ligand CLA 3 612



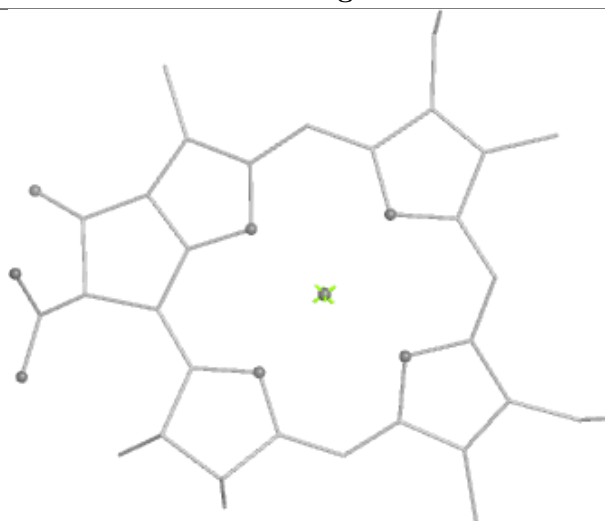
Bond lengths



Bond angles

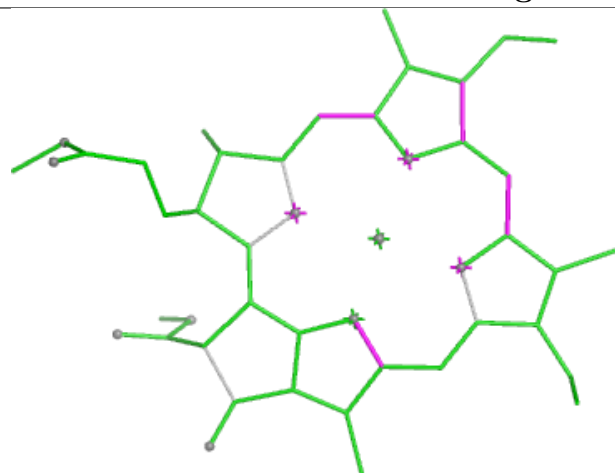


Torsions

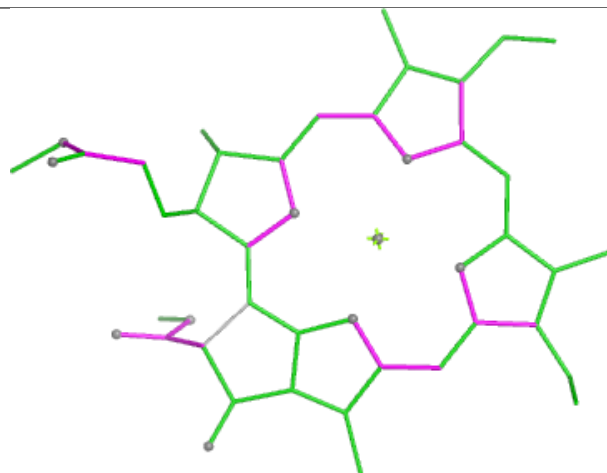


Rings

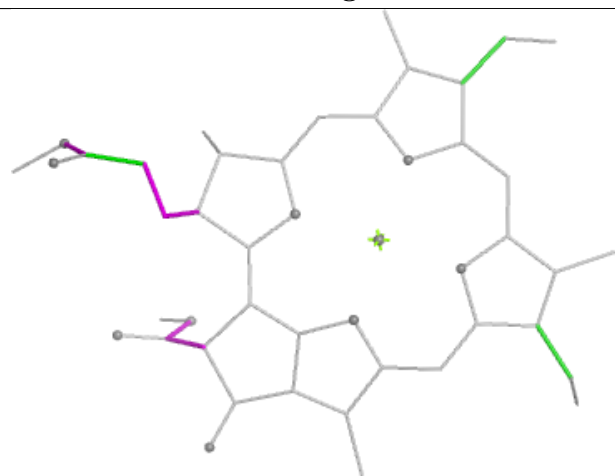
Ligand CLA K 203



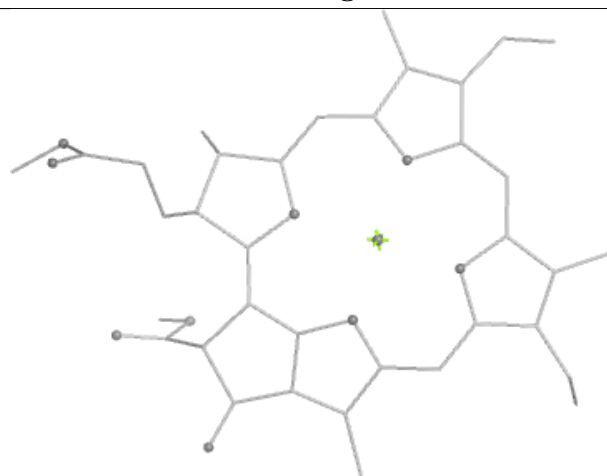
Bond lengths



Bond angles

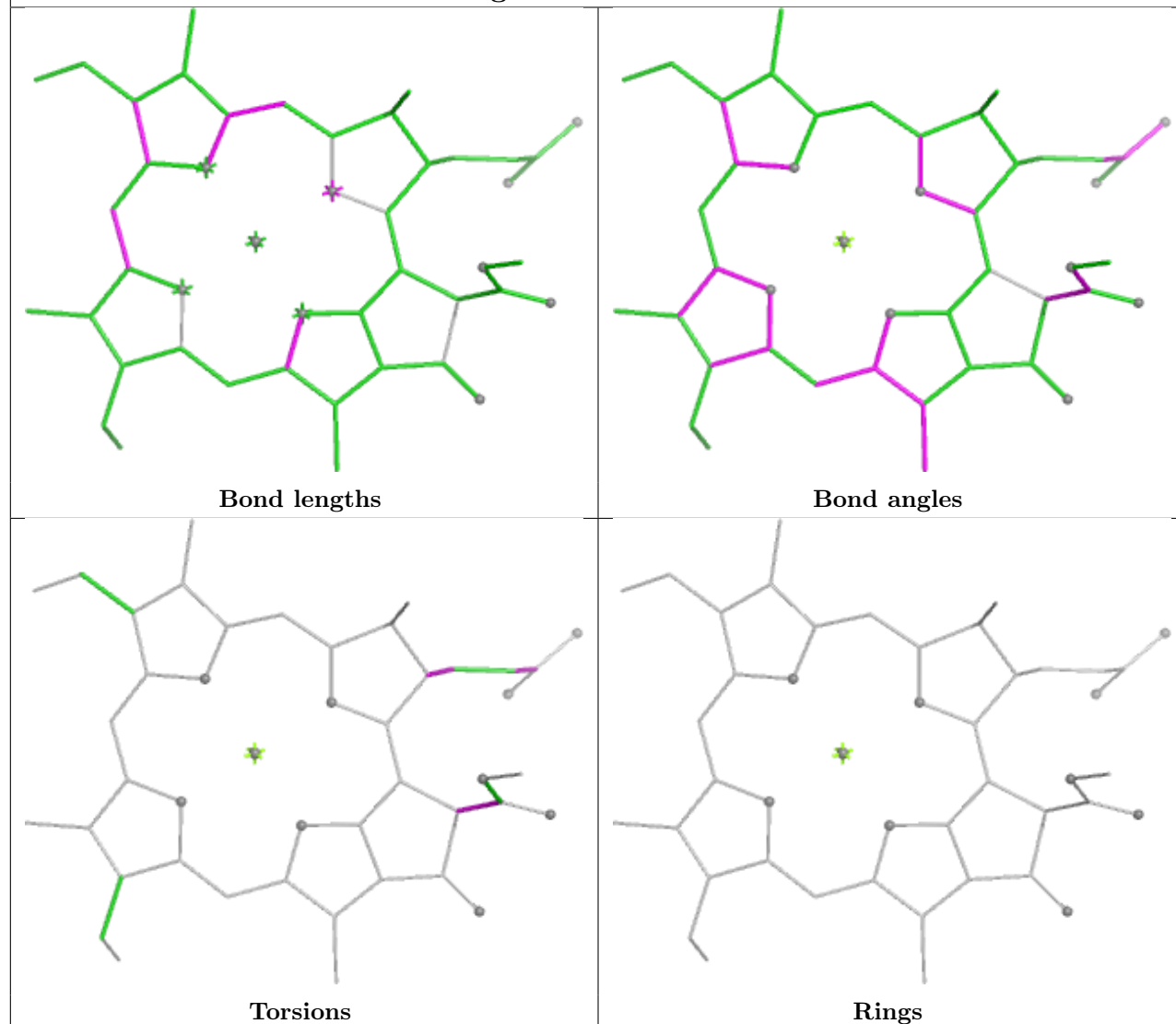


Torsions

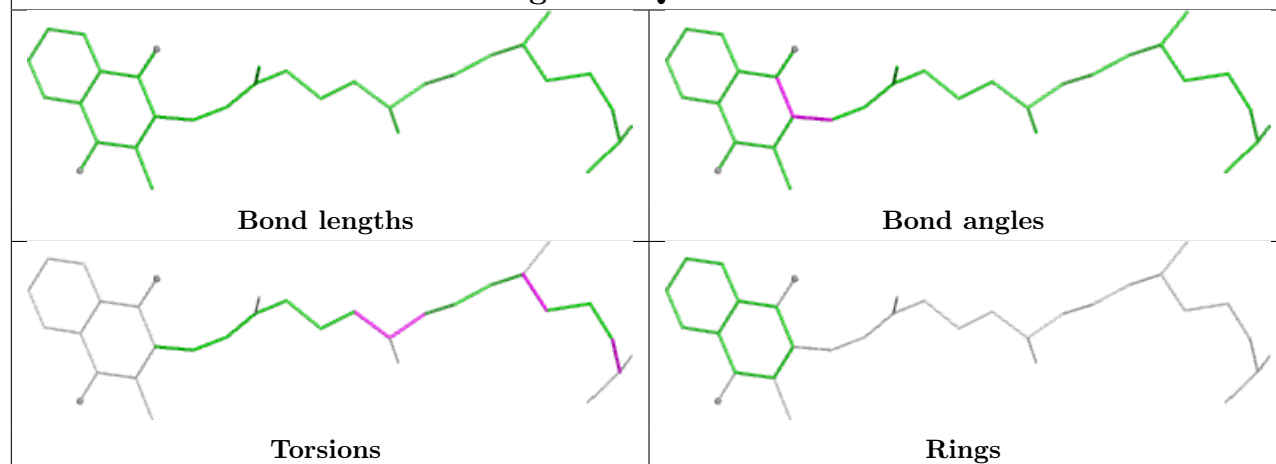


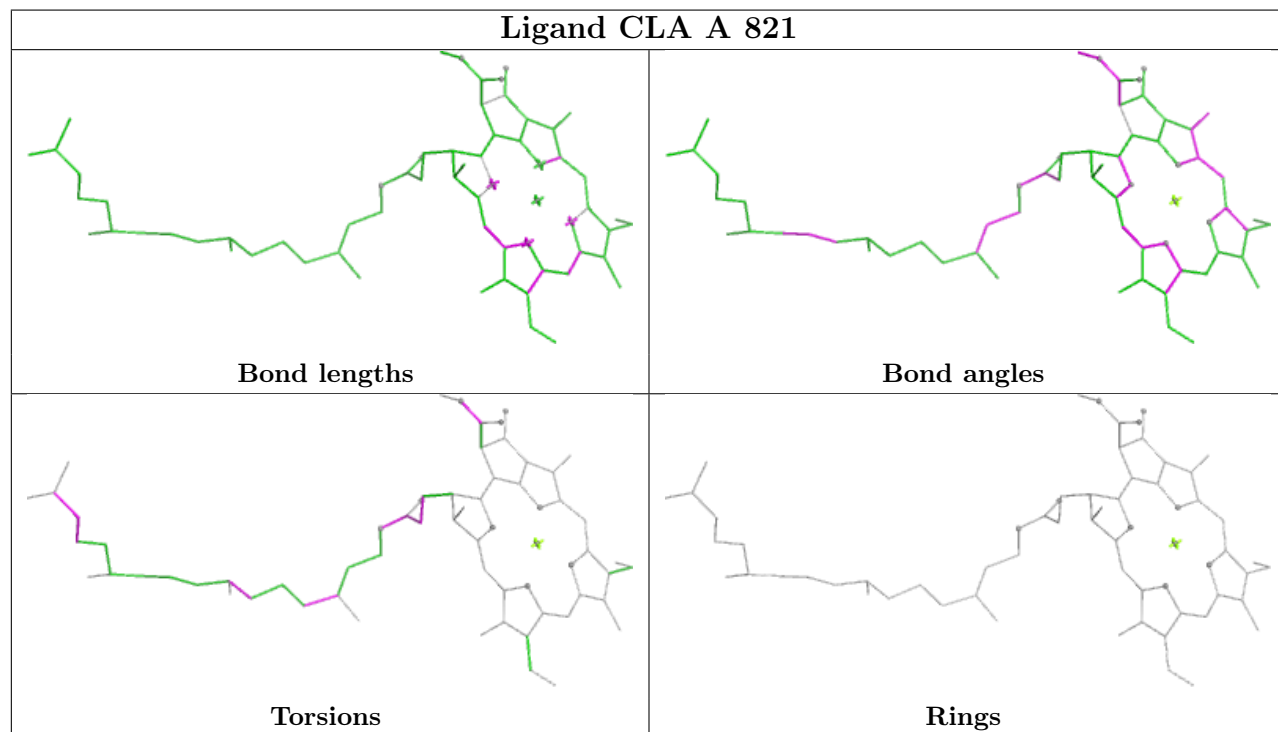
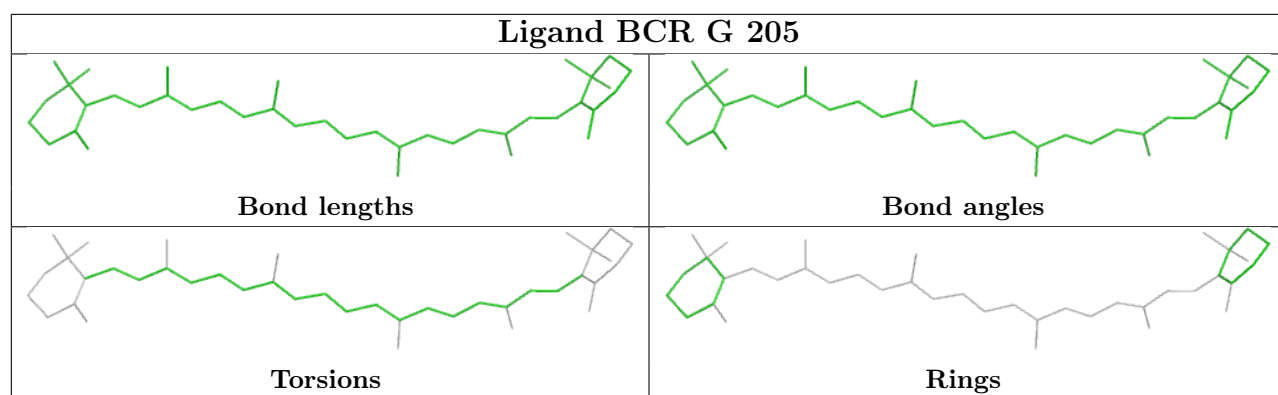
Rings

Ligand CLA B 832

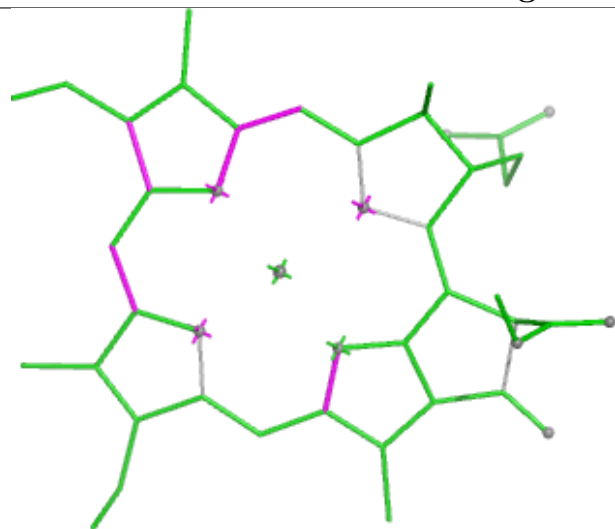


Ligand PQN A 844

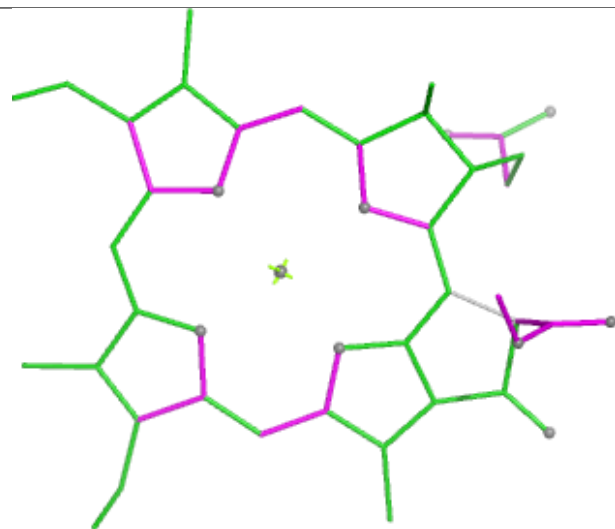




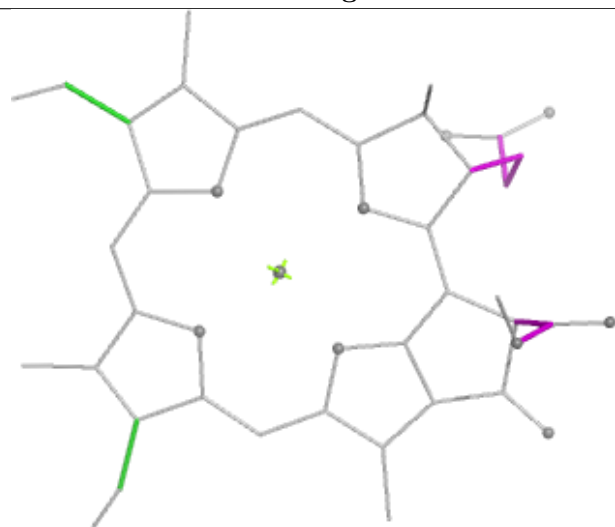
Ligand CLA L 304



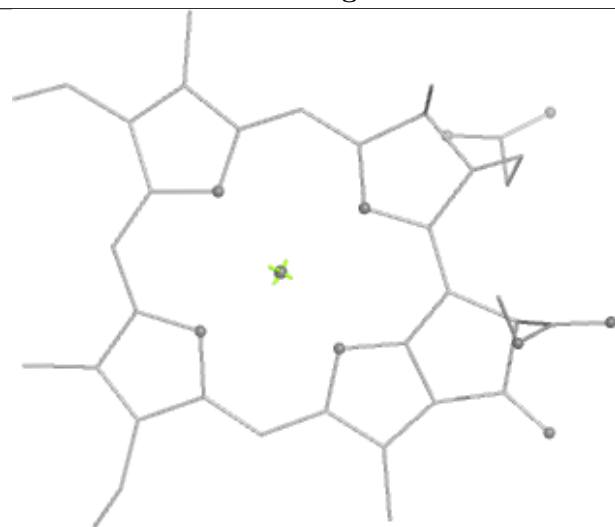
Bond lengths



Bond angles

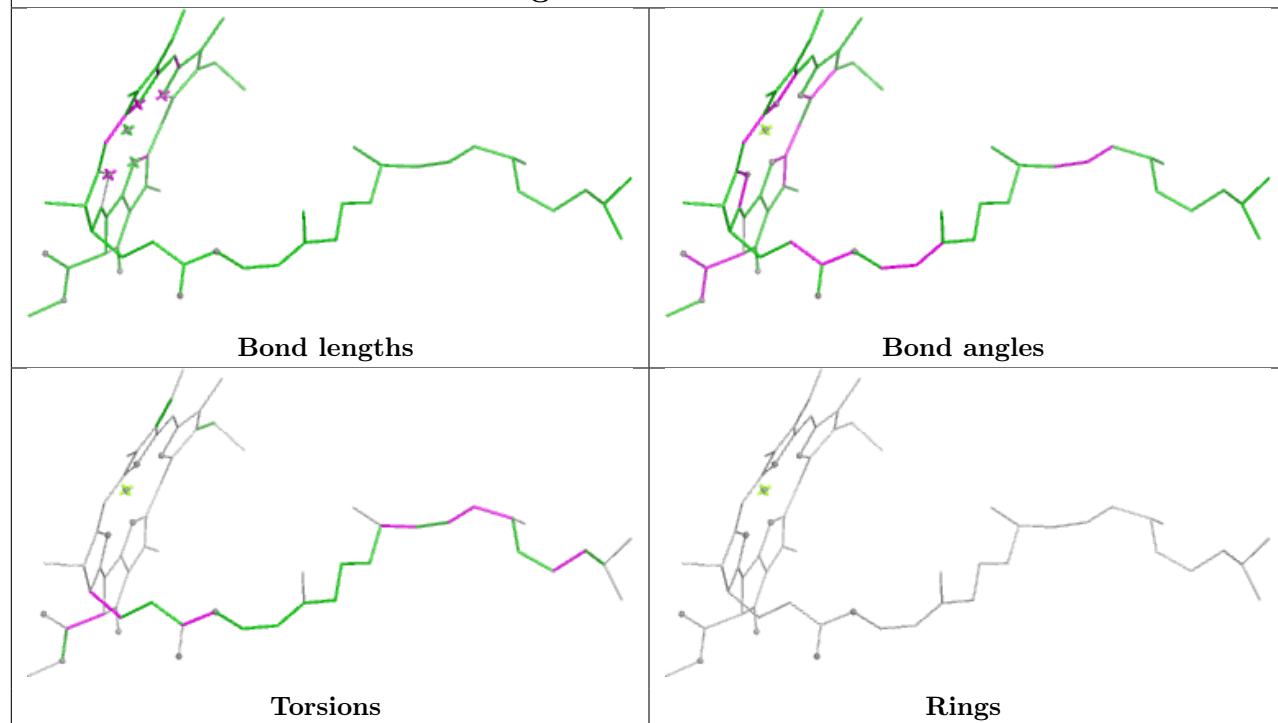


Torsions

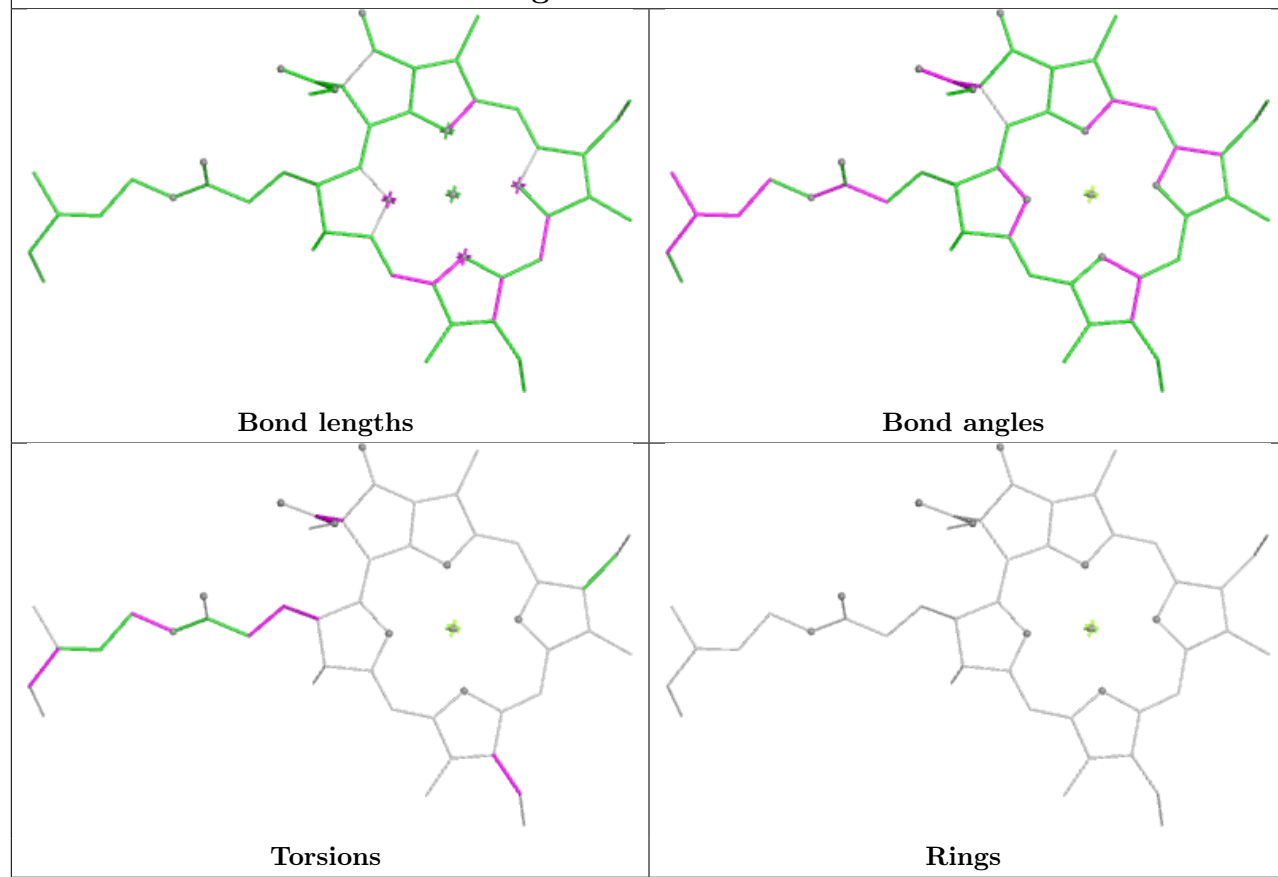


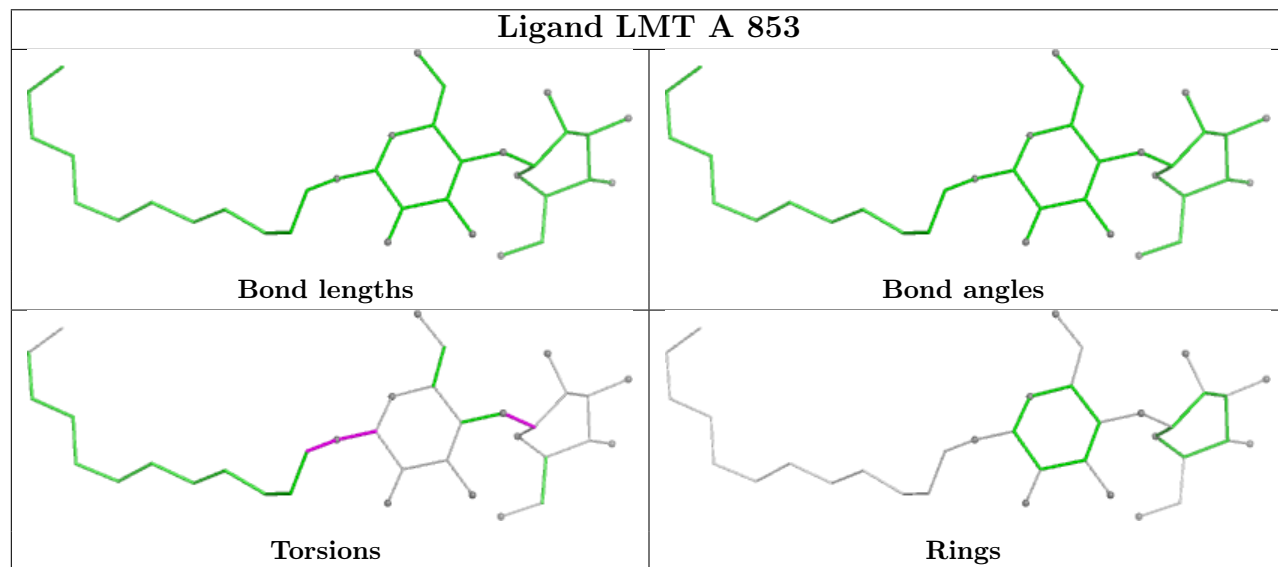
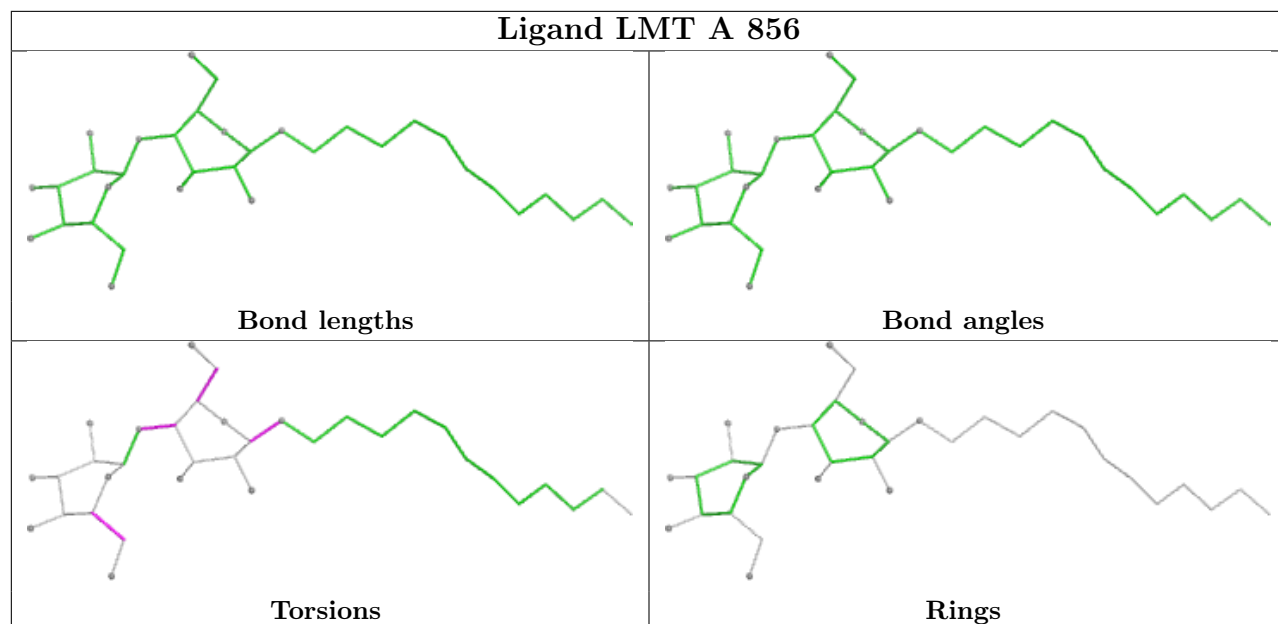
Rings

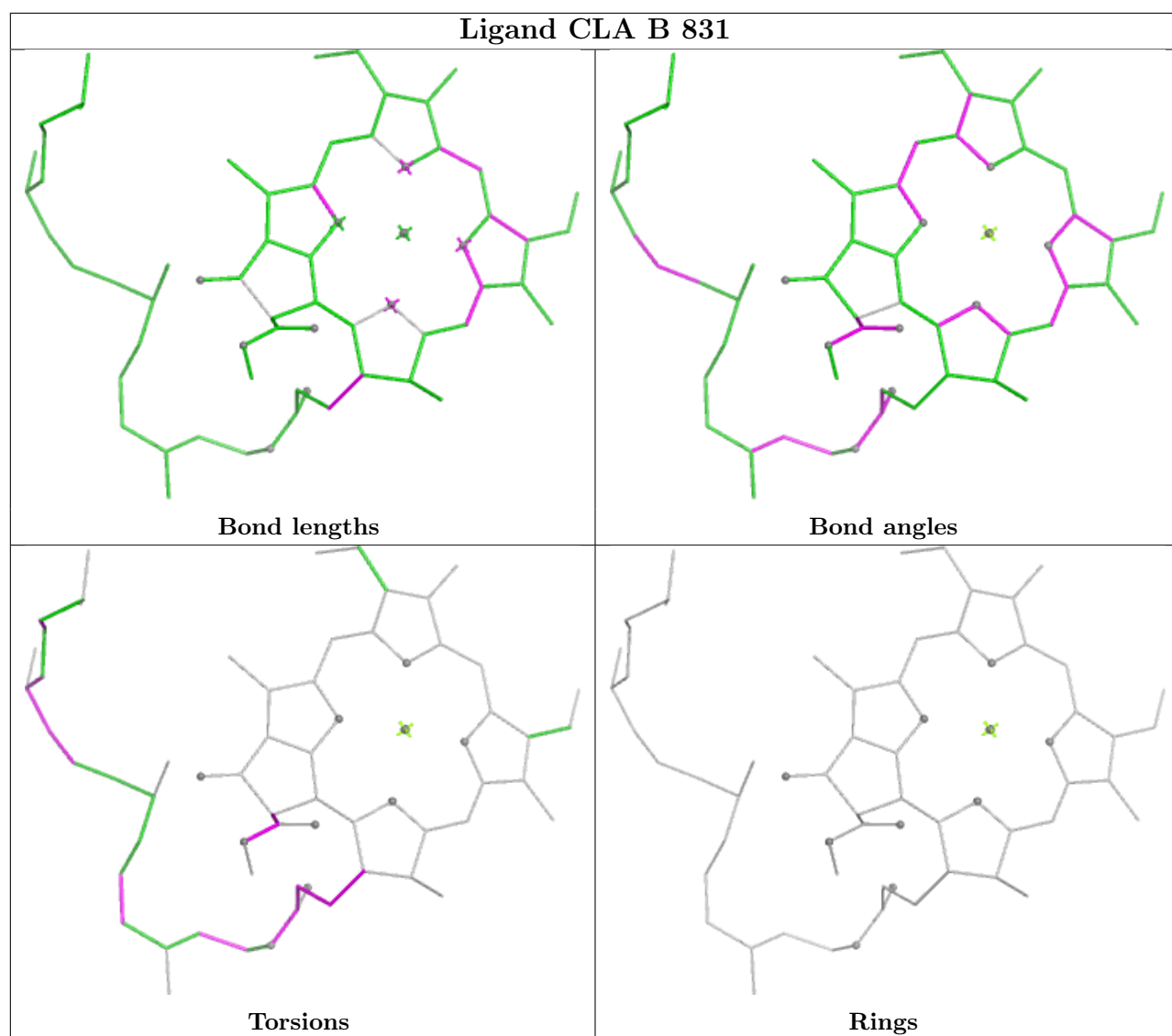
Ligand CLA A 811



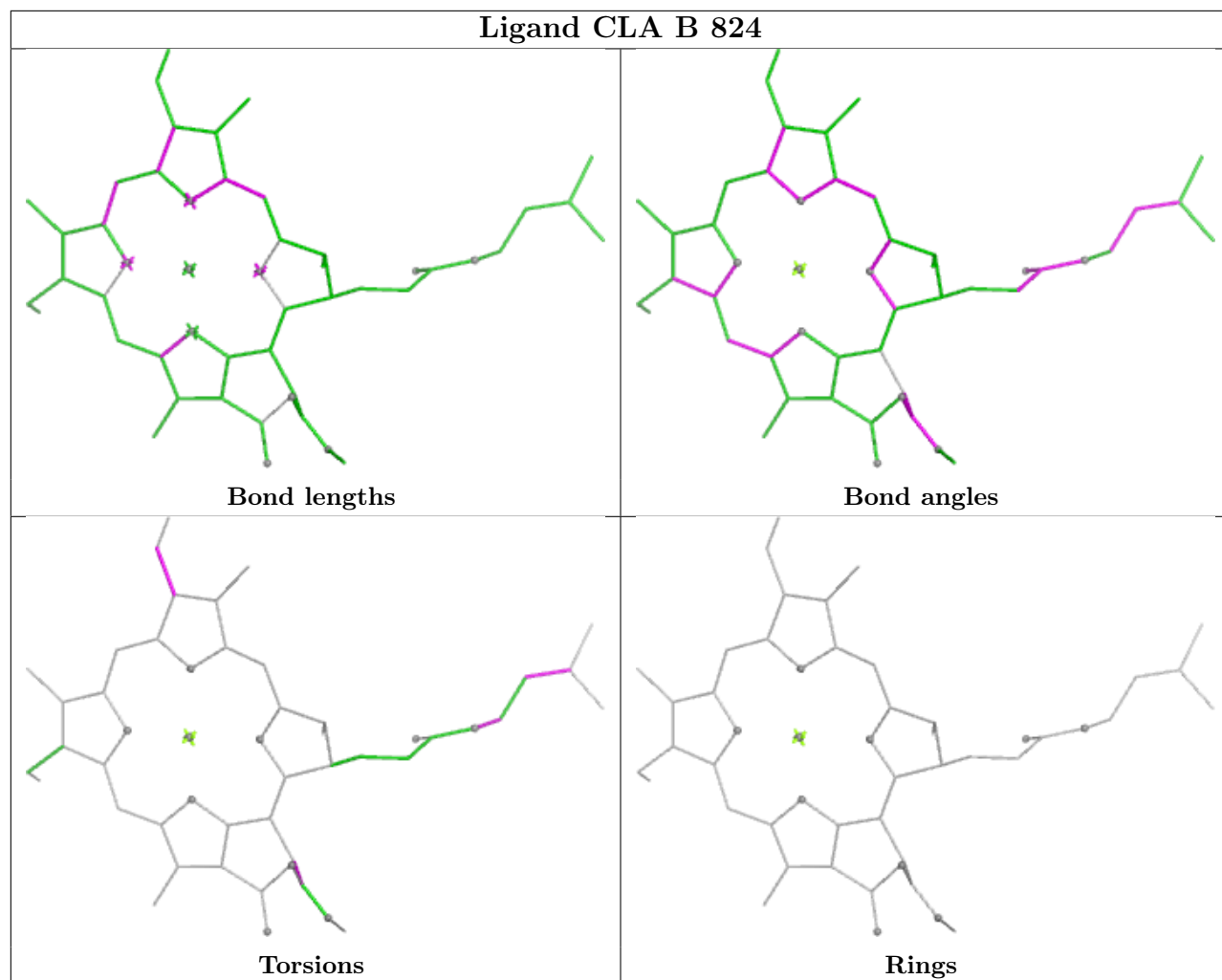
Ligand CLA A 837



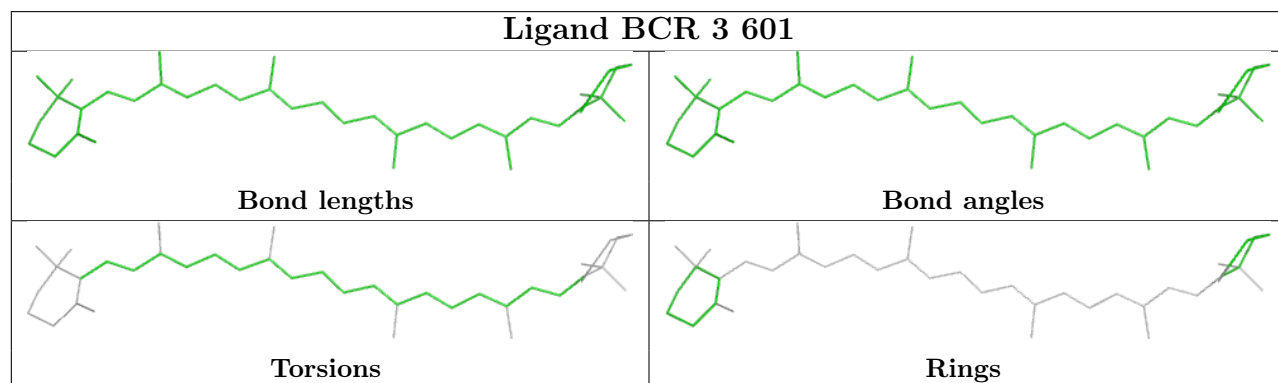




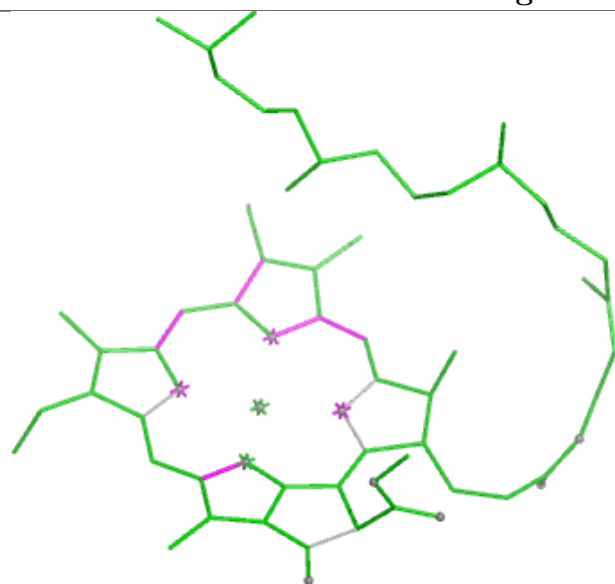
Ligand CLA B 824



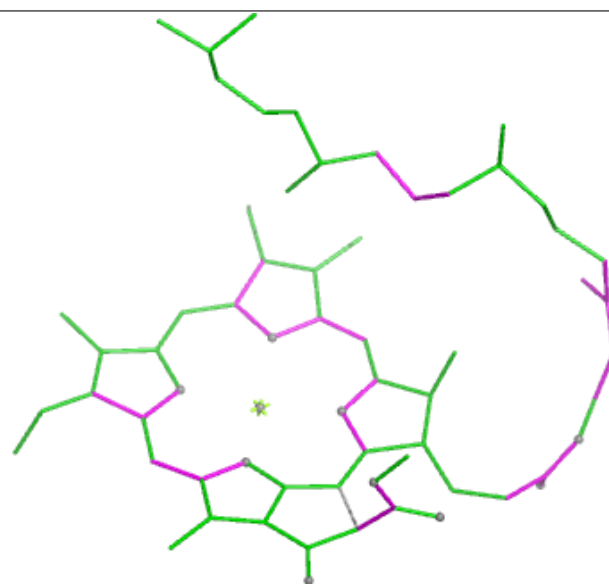
Ligand BCR 3 601



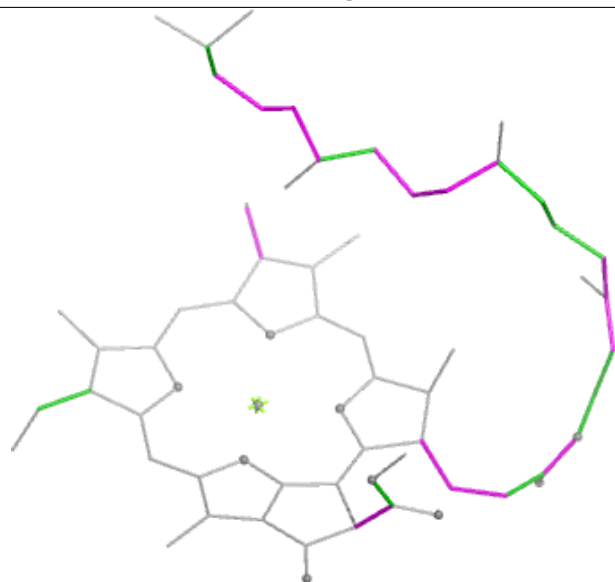
Ligand CLA A 813



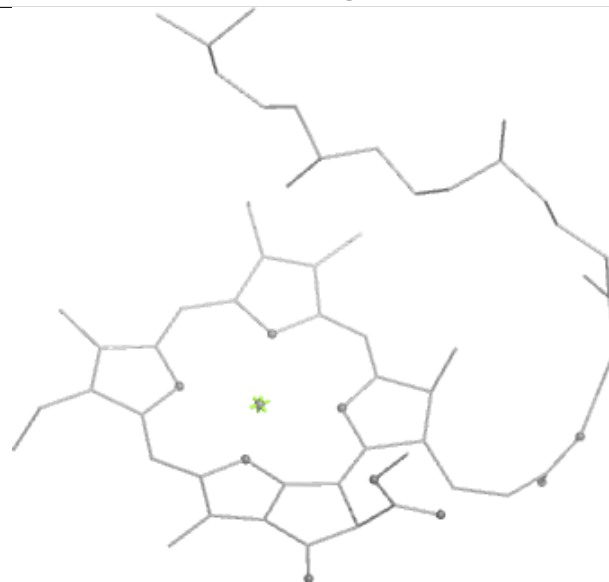
Bond lengths



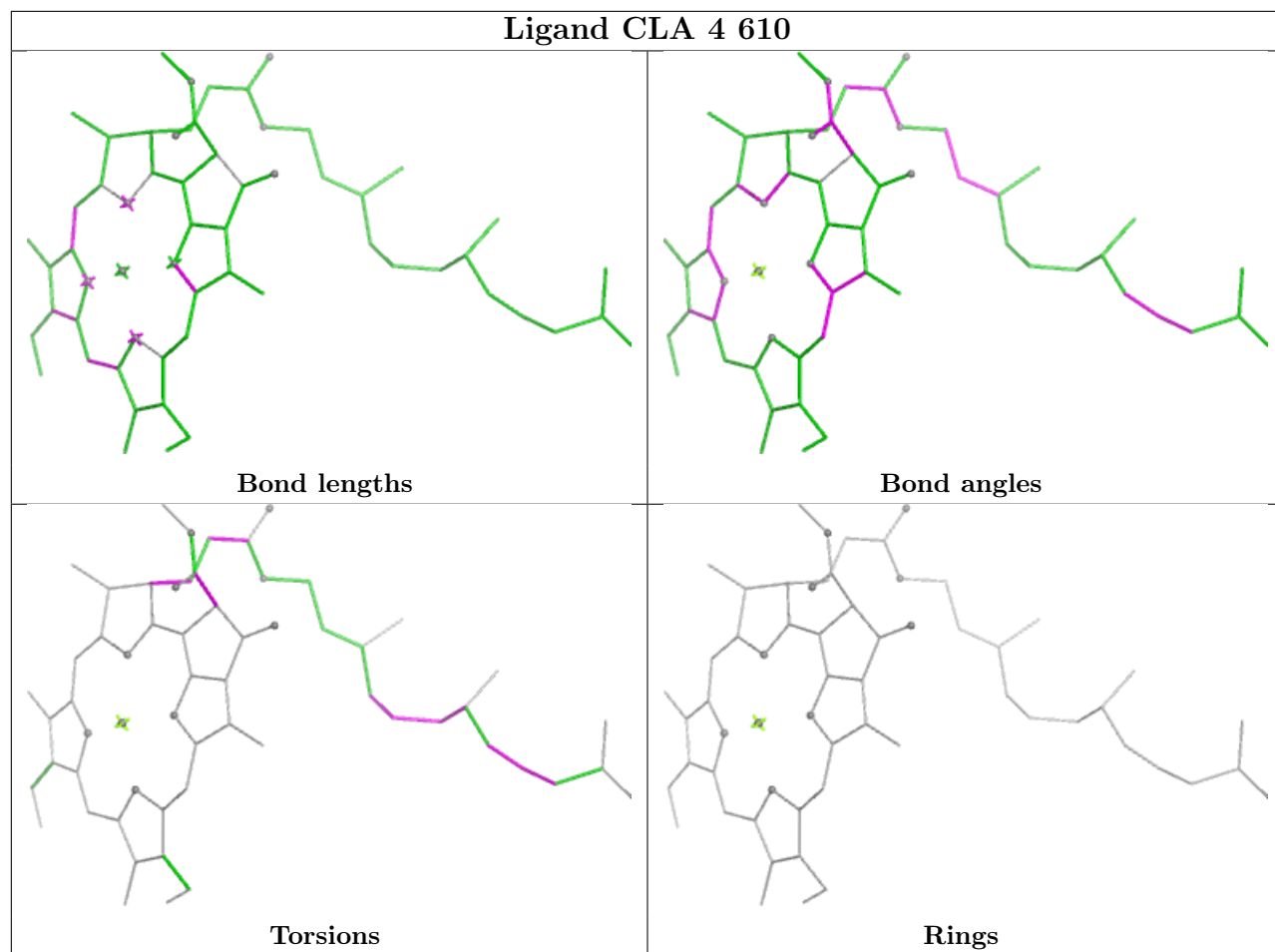
Bond angles



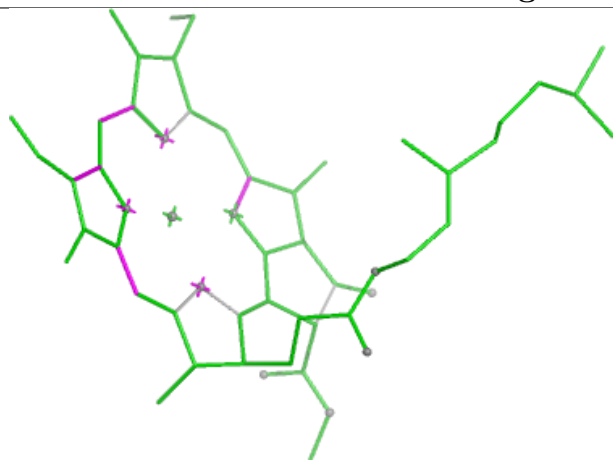
Torsions



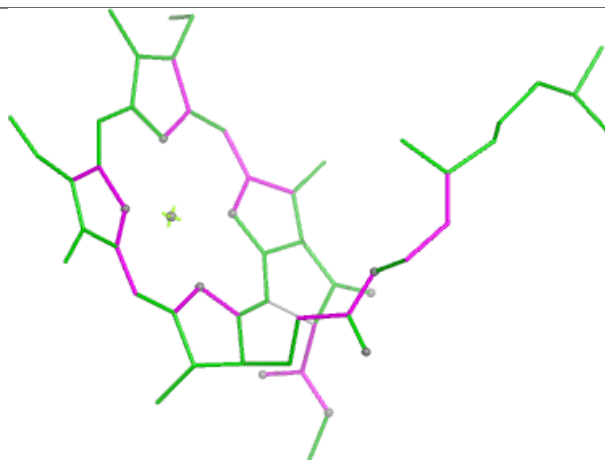
Rings



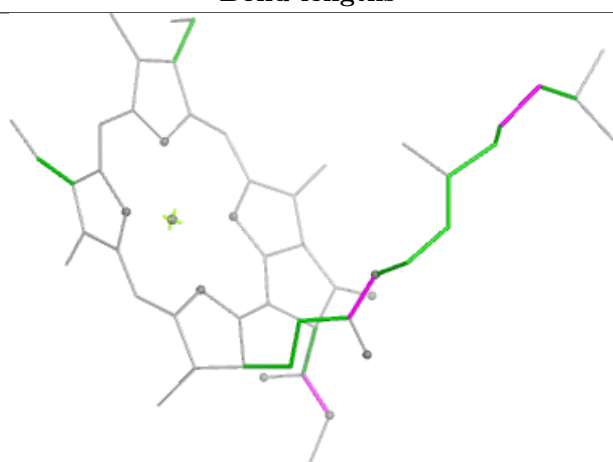
Ligand CLA 1 610



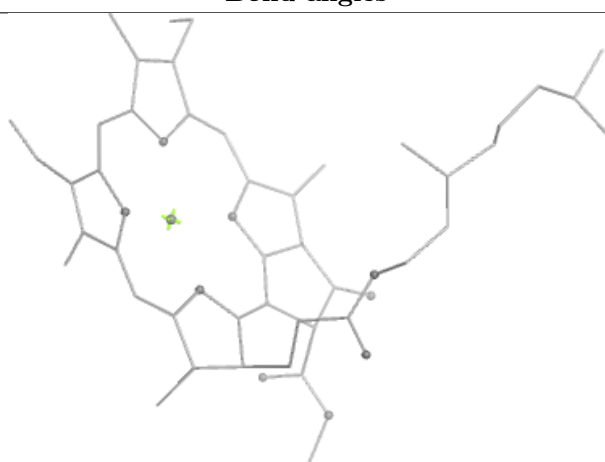
Bond lengths



Bond angles

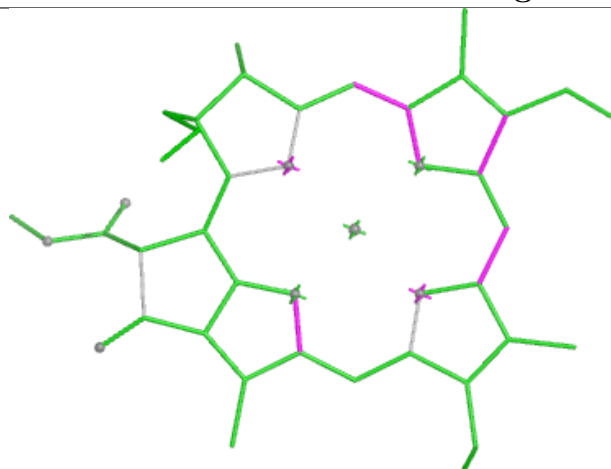


Torsions

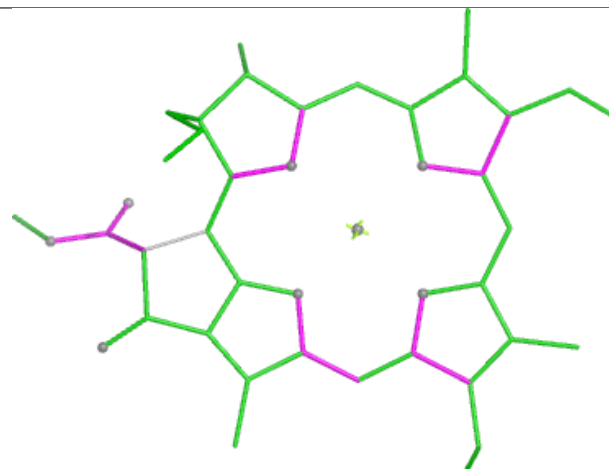


Rings

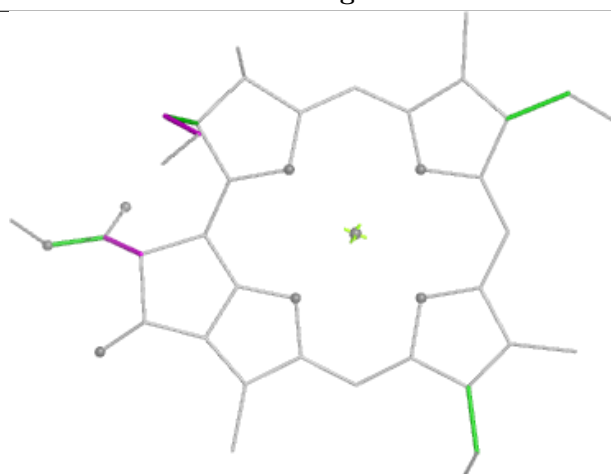
Ligand CLA B 811



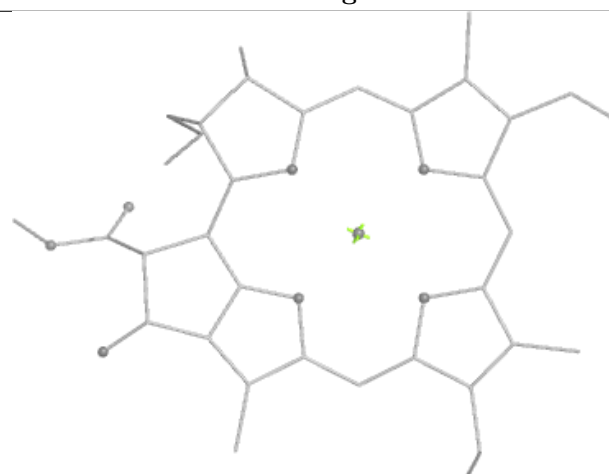
Bond lengths



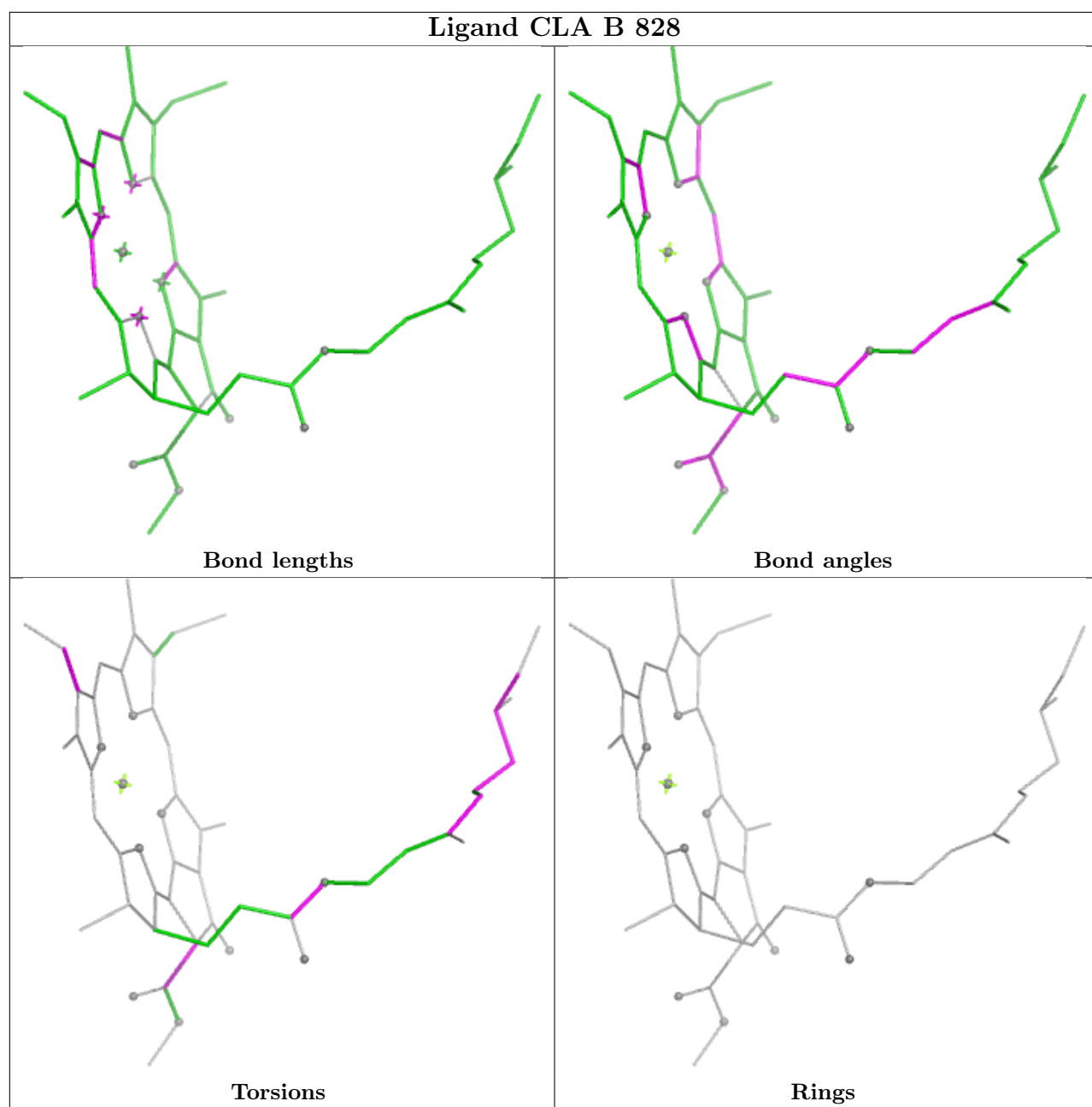
Bond angles

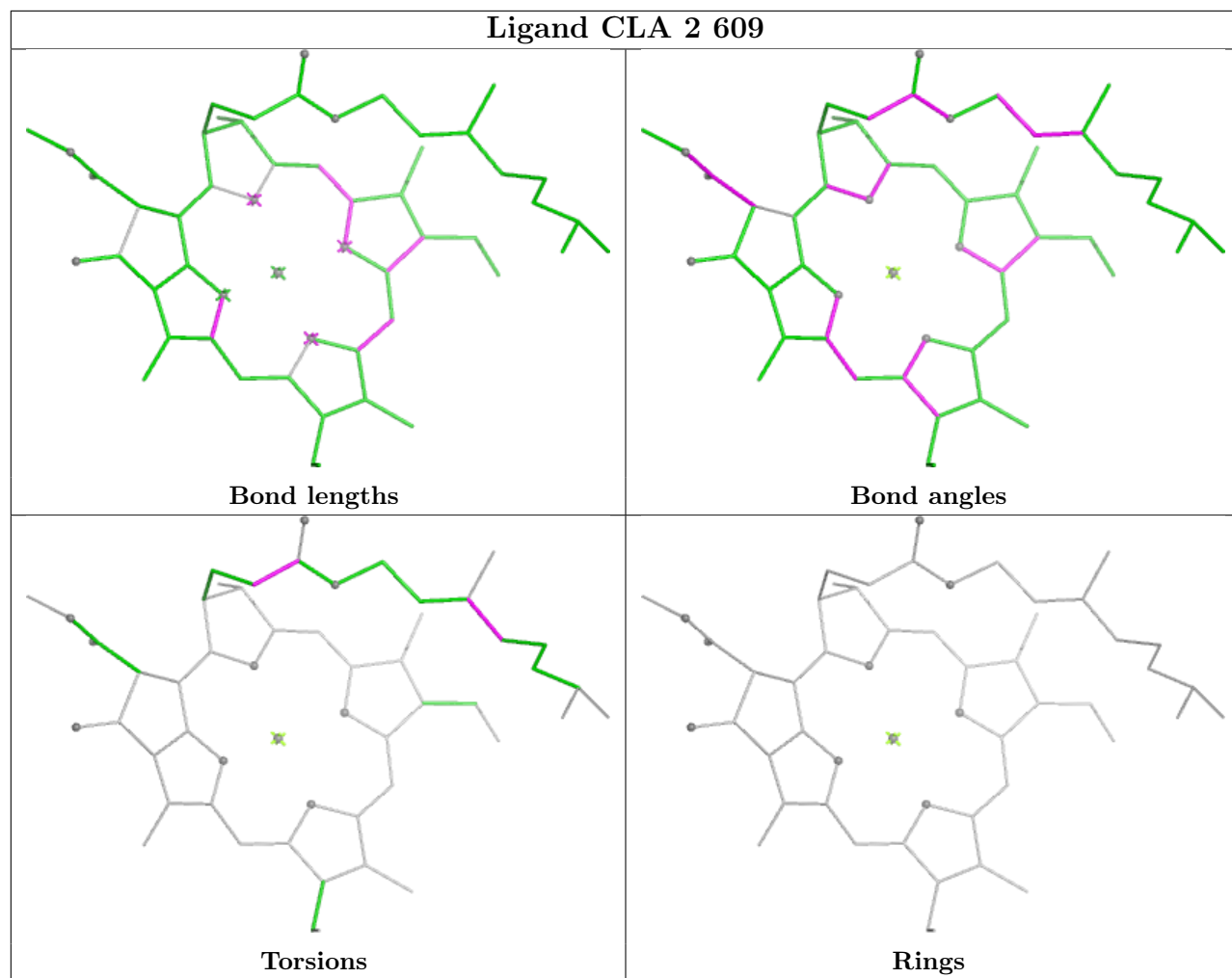


Torsions

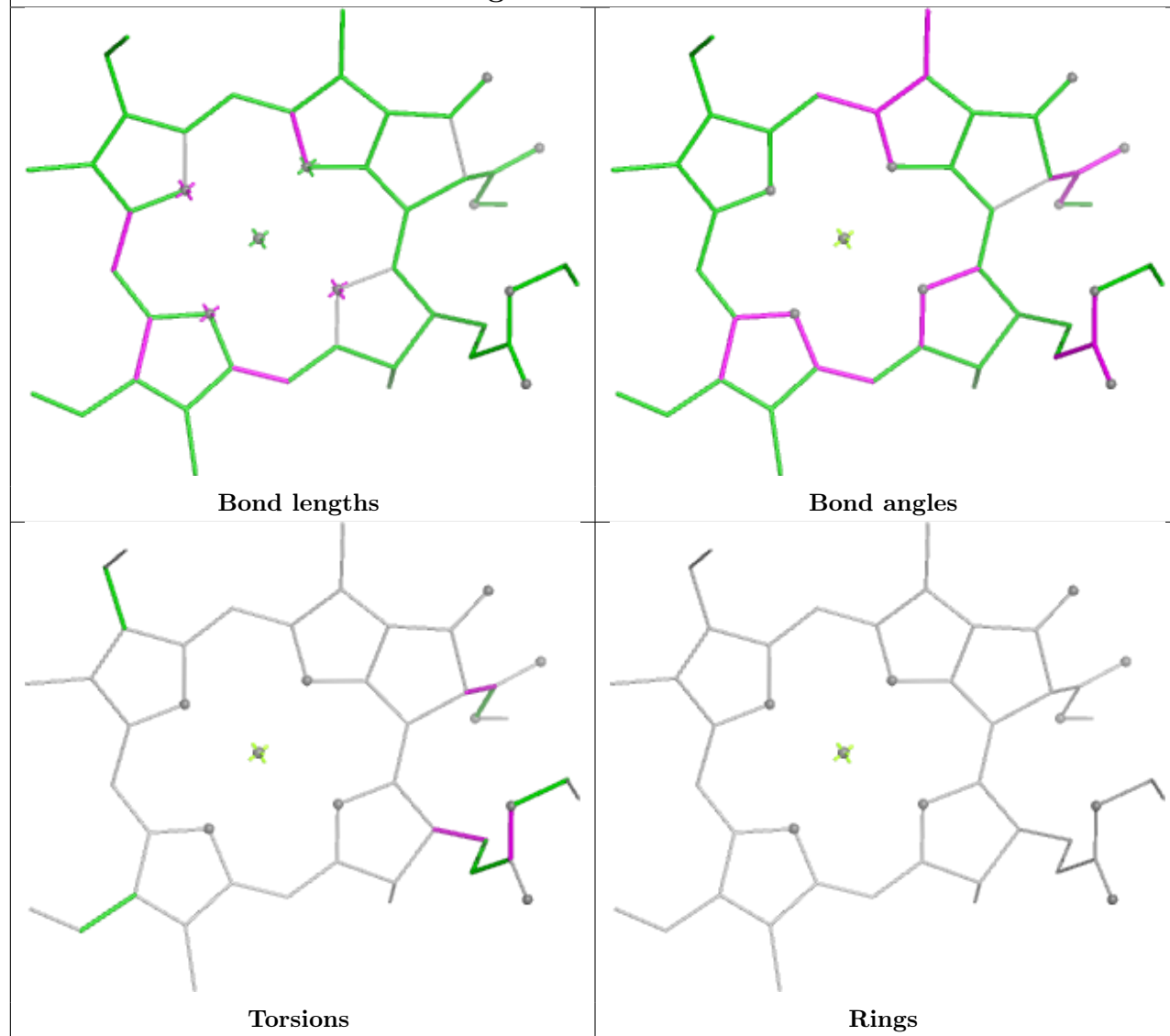


Rings

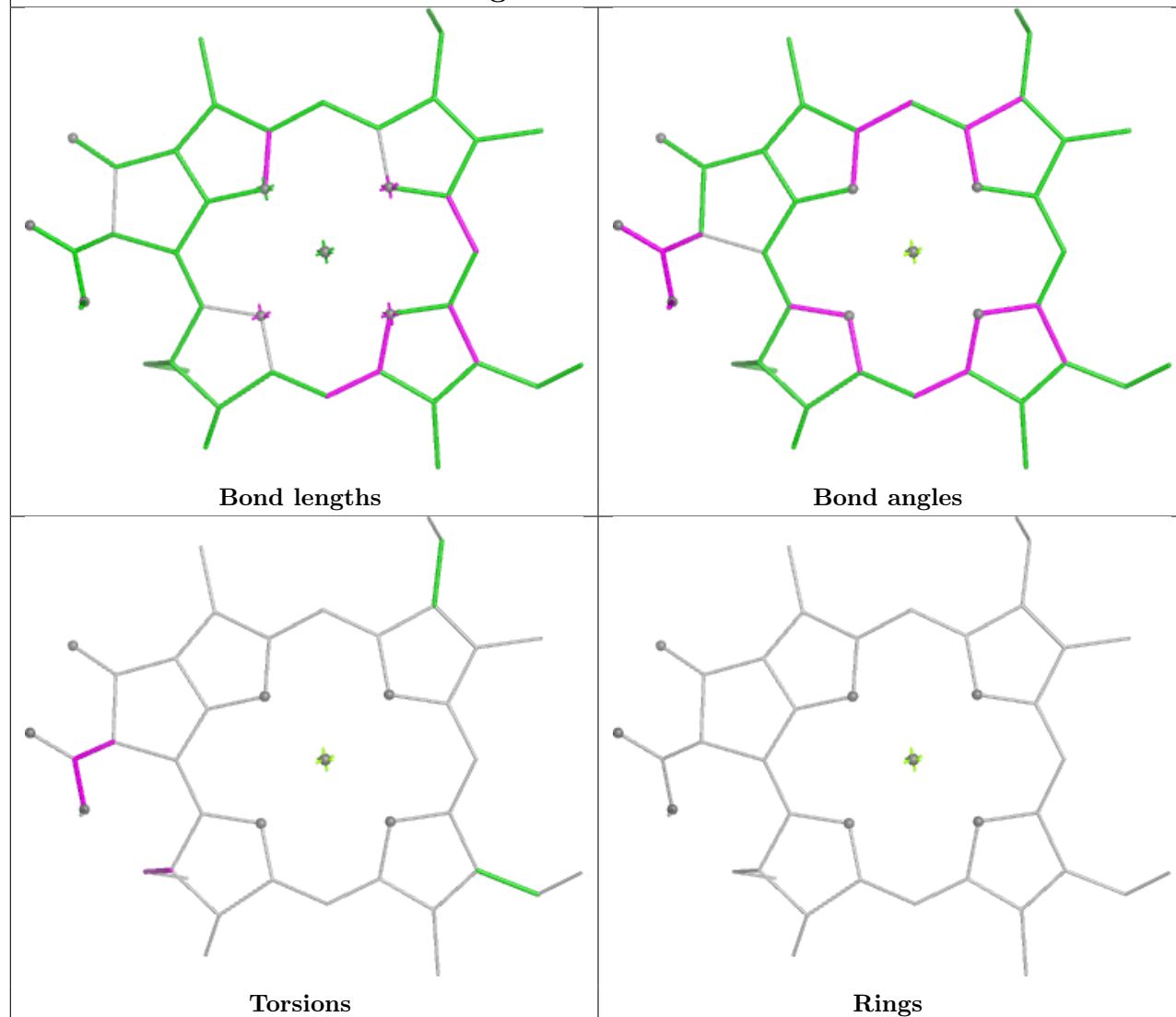




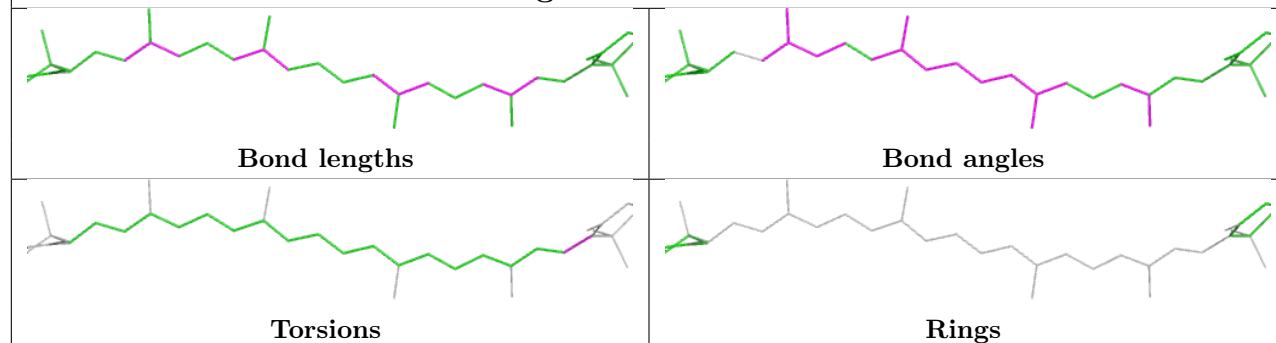
Ligand CLA B 837

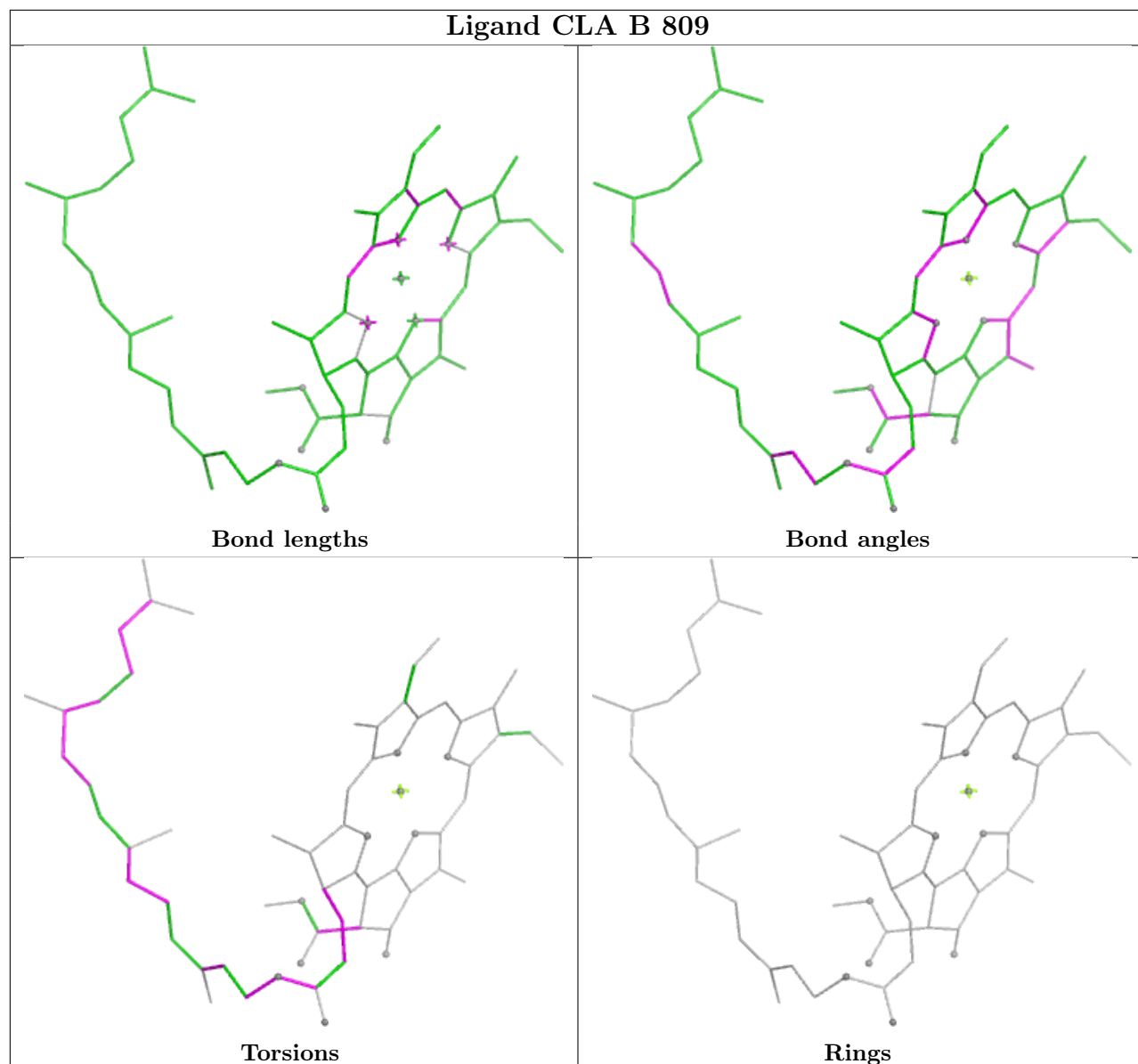
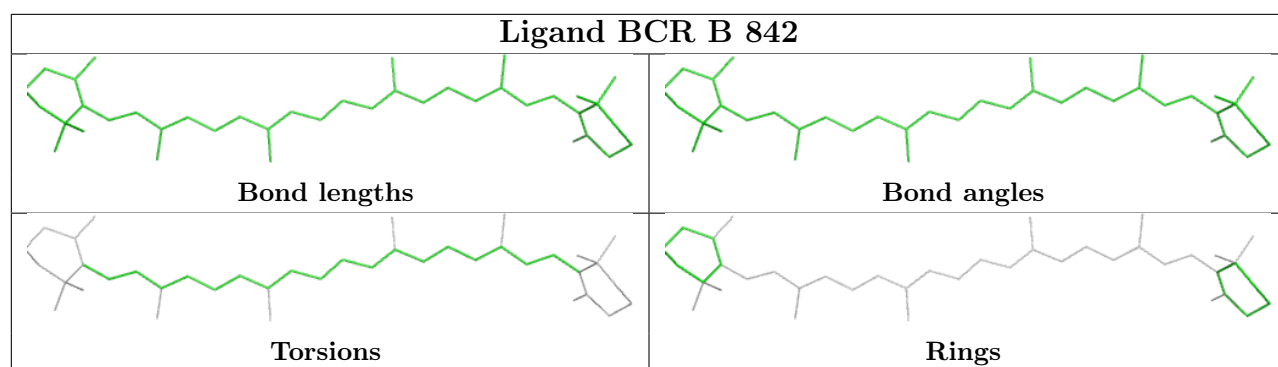


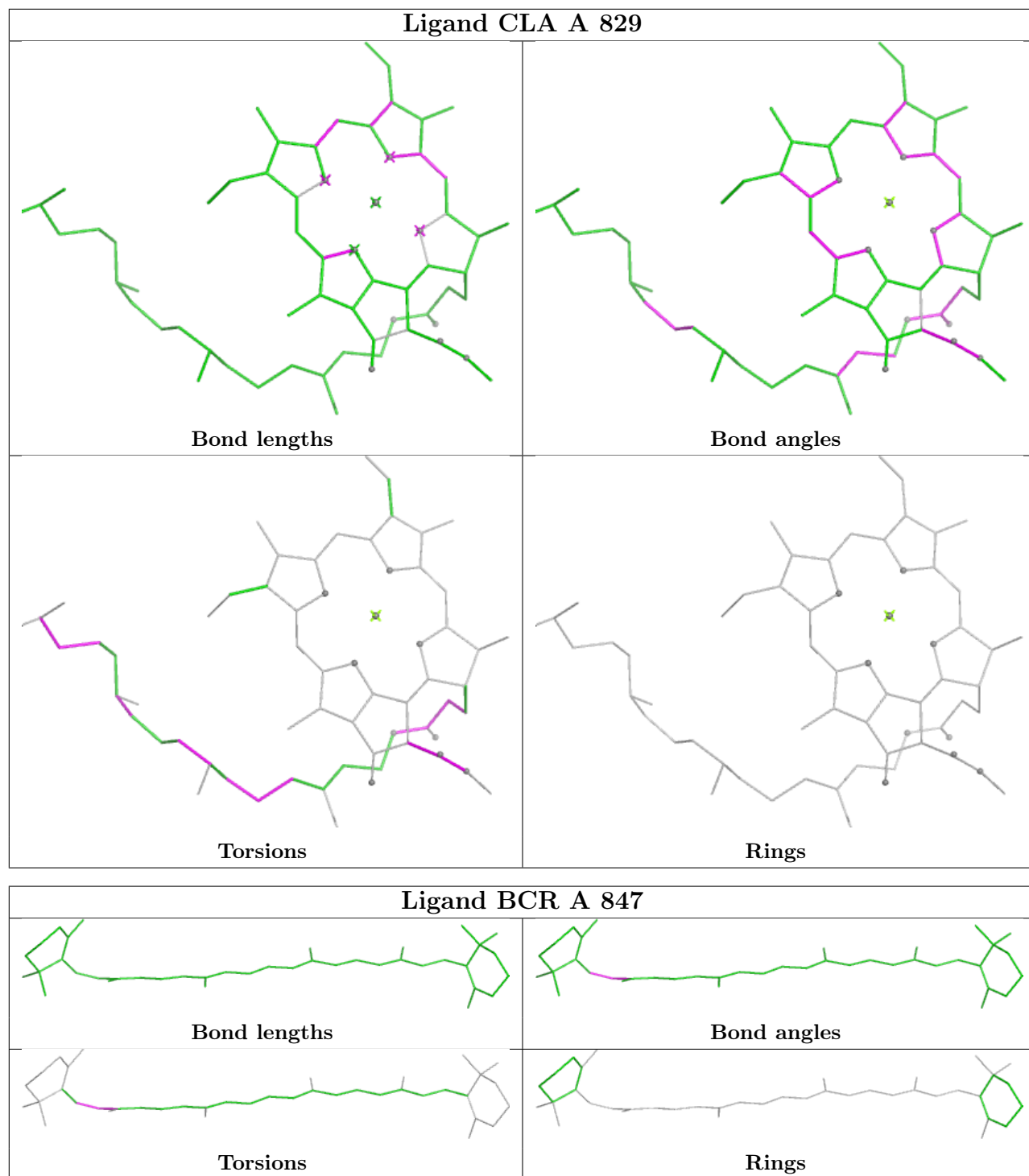
Ligand CLA A 822



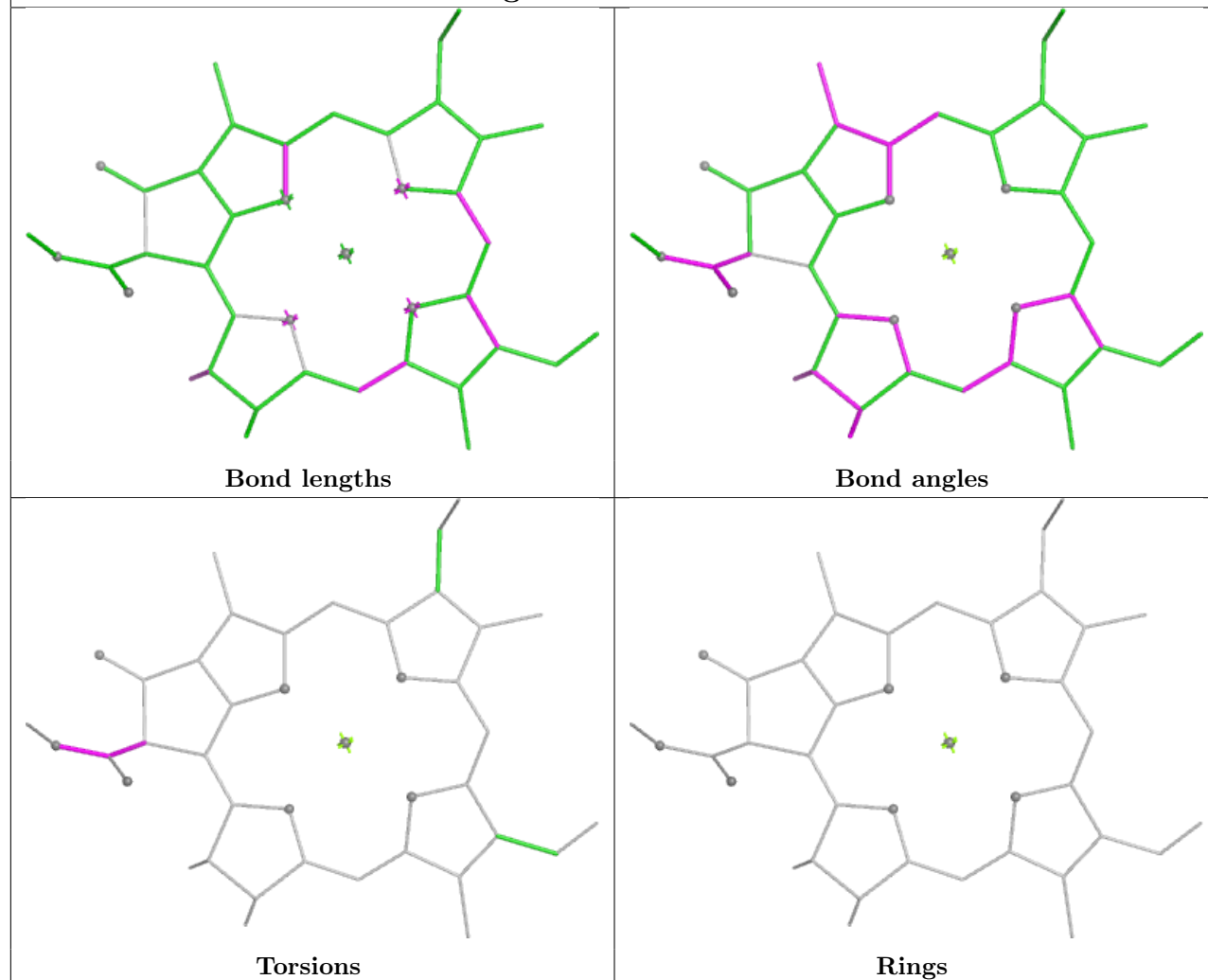
Ligand LUT 2 615



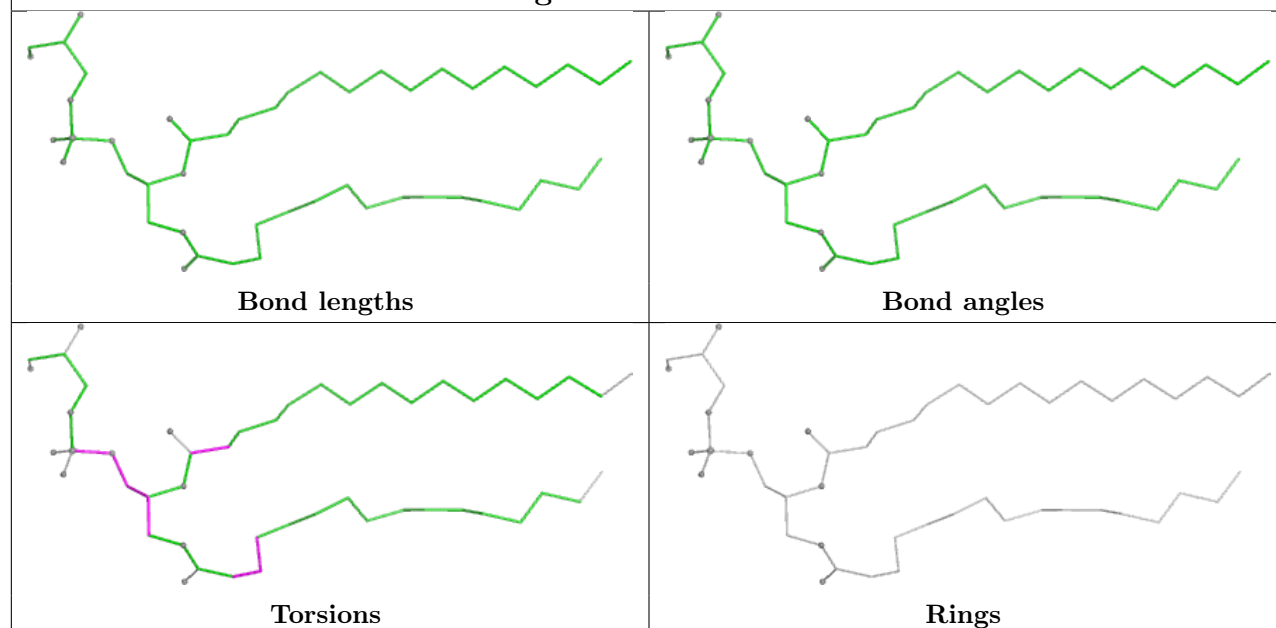


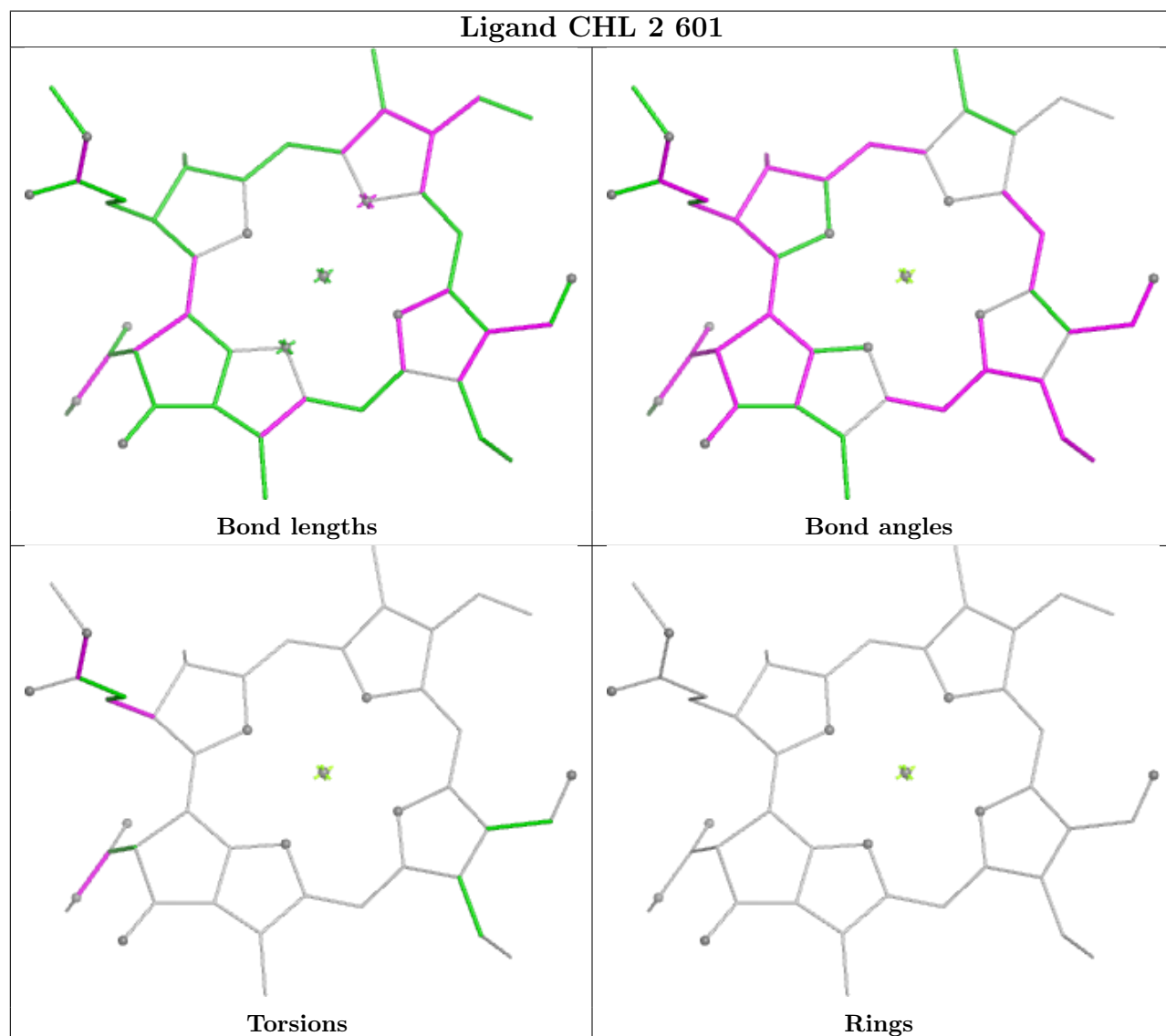
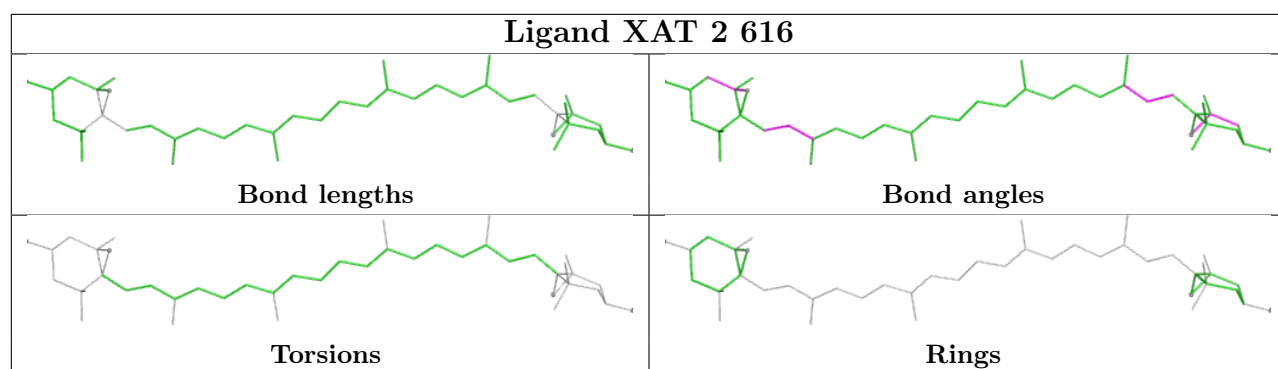


Ligand CLA A 823

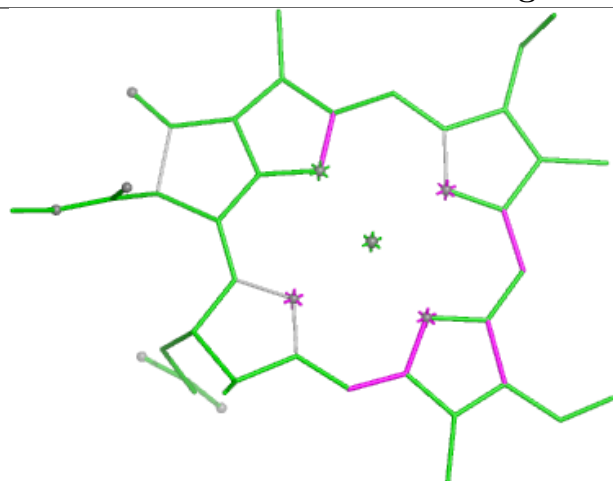


Ligand LHG 1 618

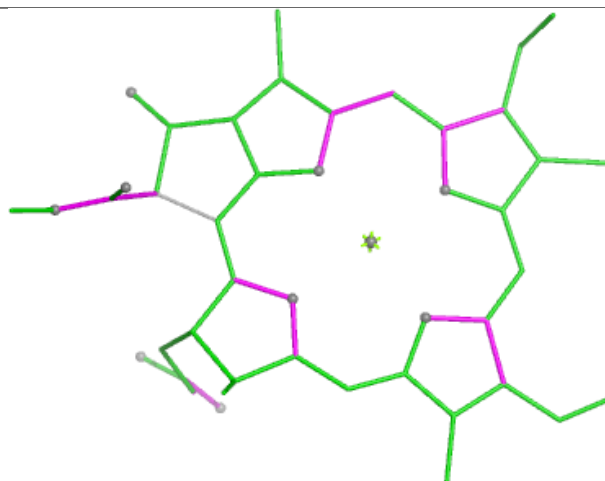




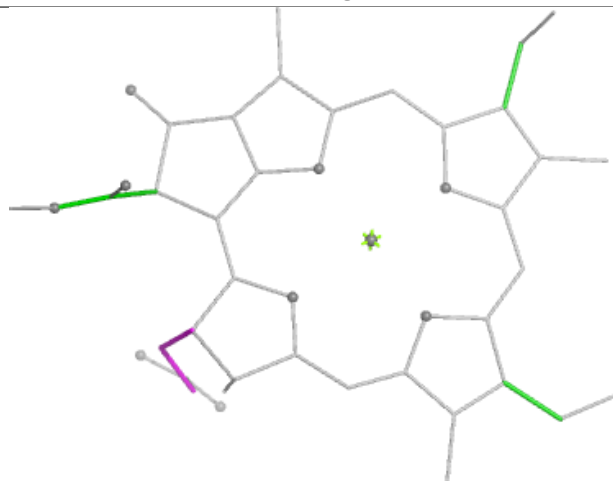
Ligand CLA 4 608



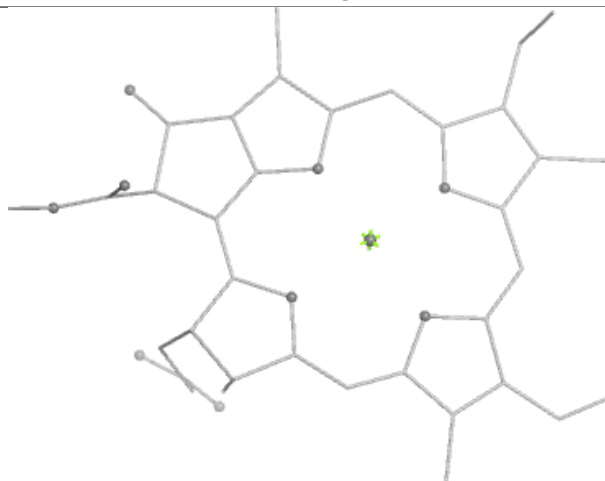
Bond lengths



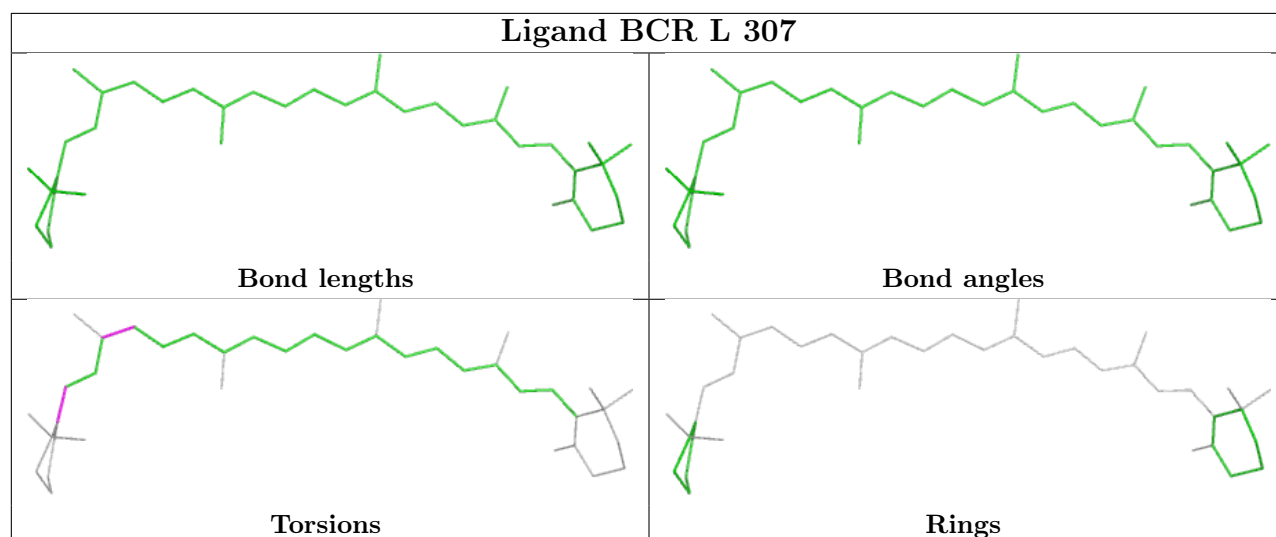
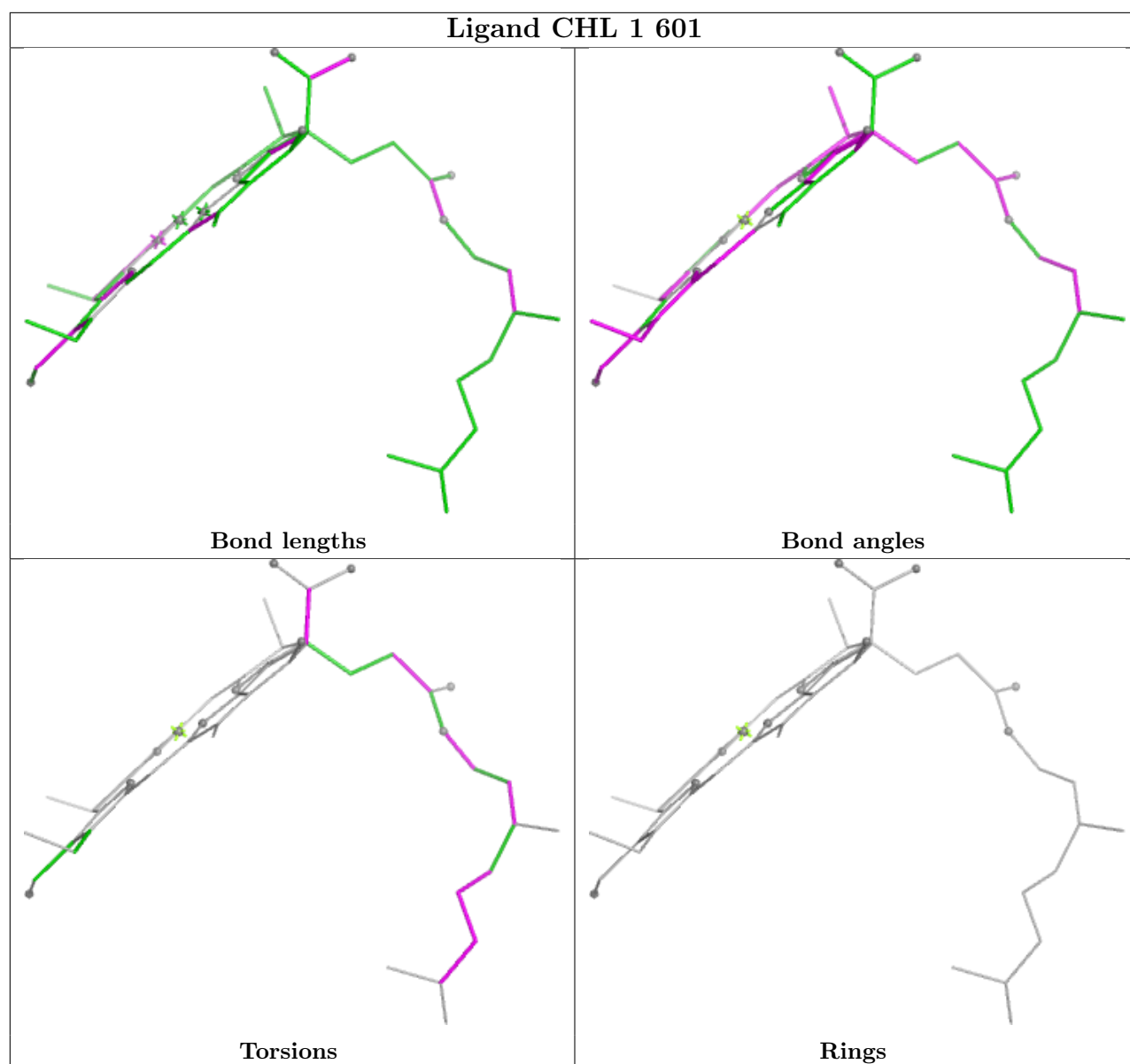
Bond angles

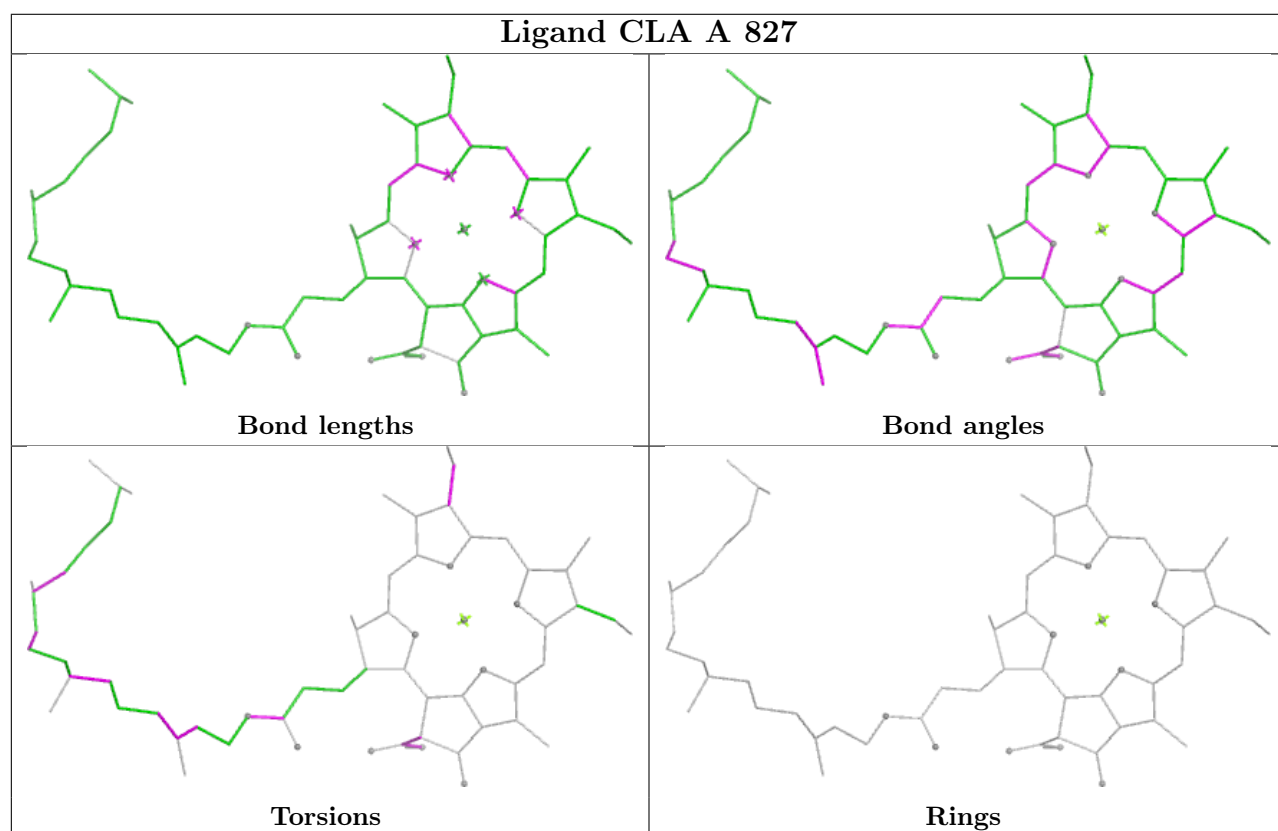
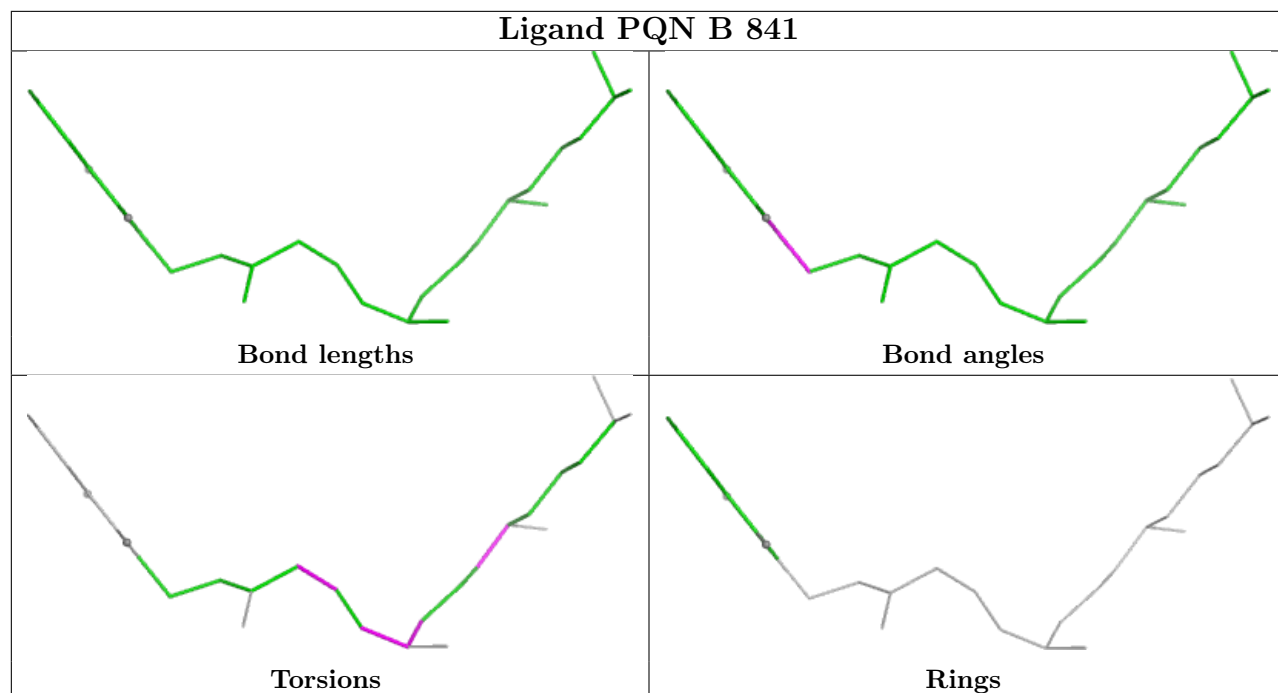


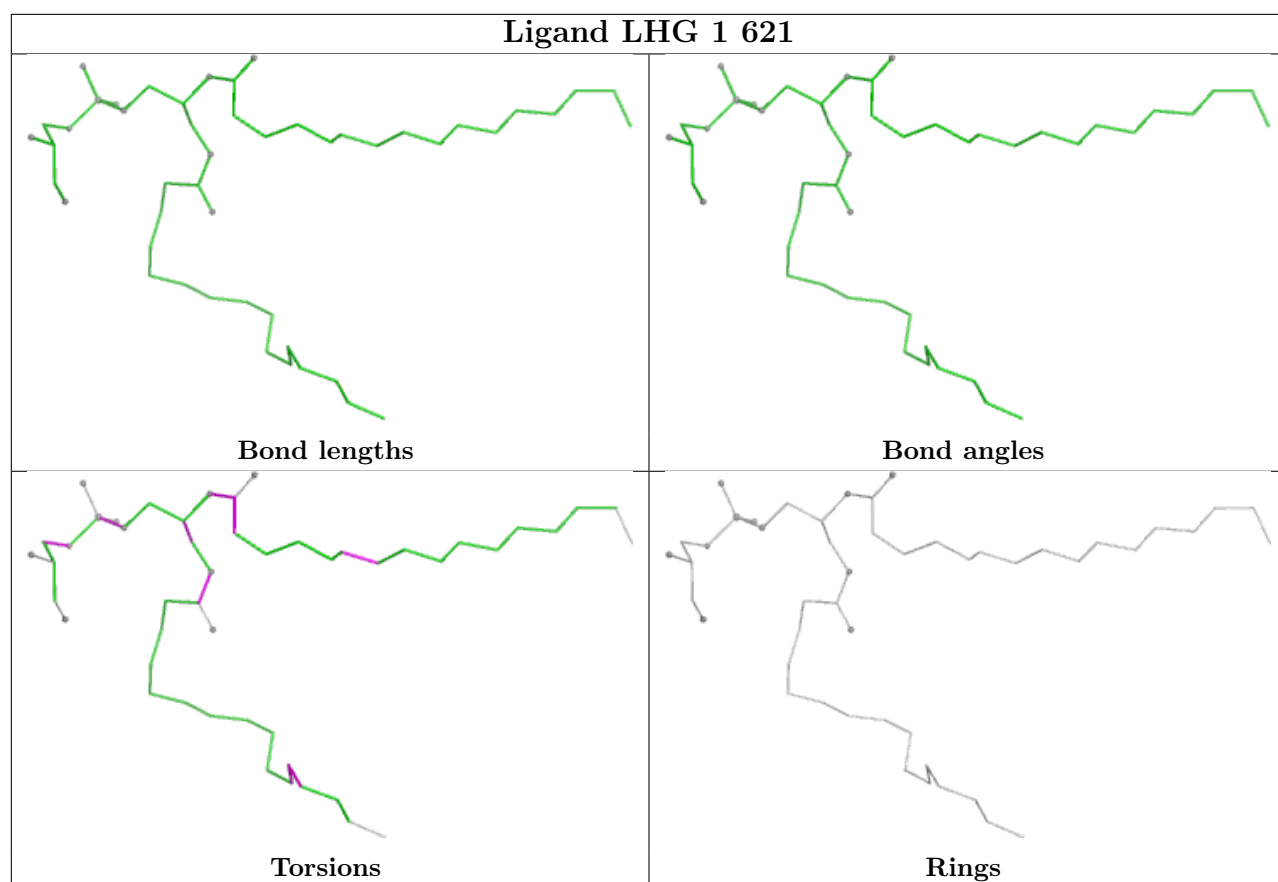
Torsions



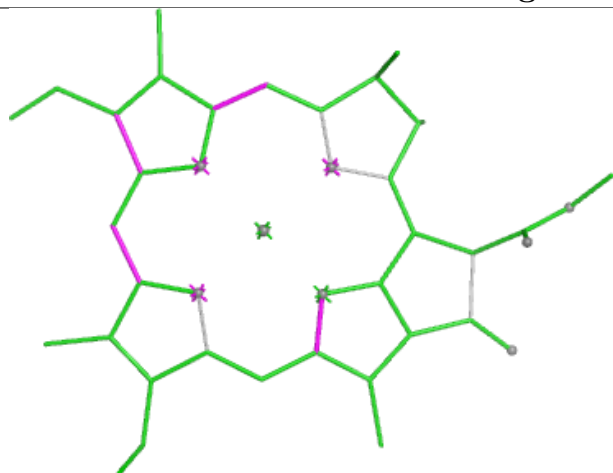
Rings



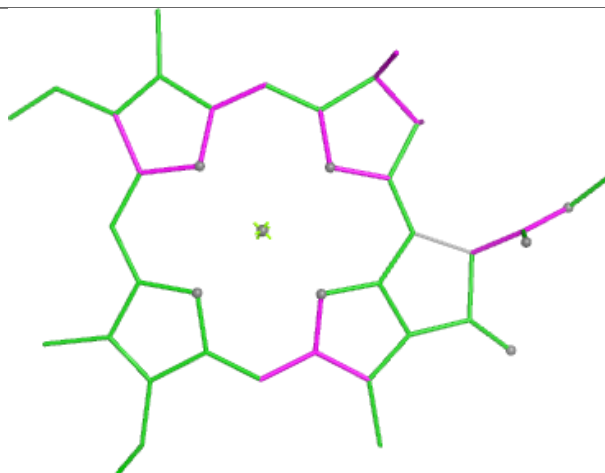




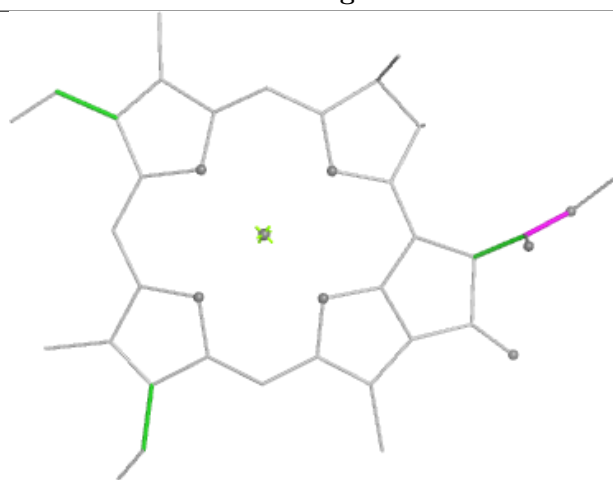
Ligand CLA 2 610



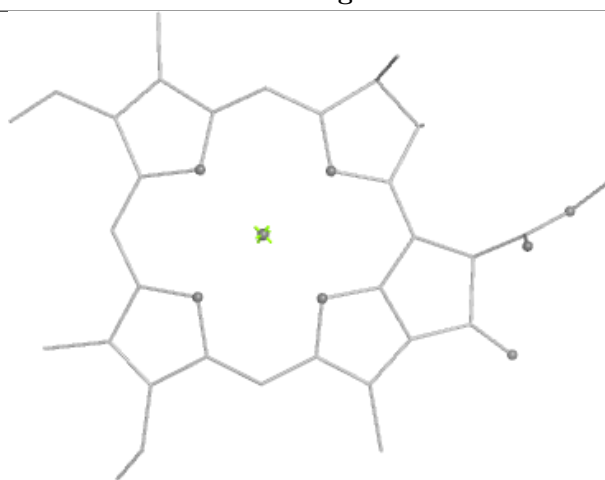
Bond lengths



Bond angles

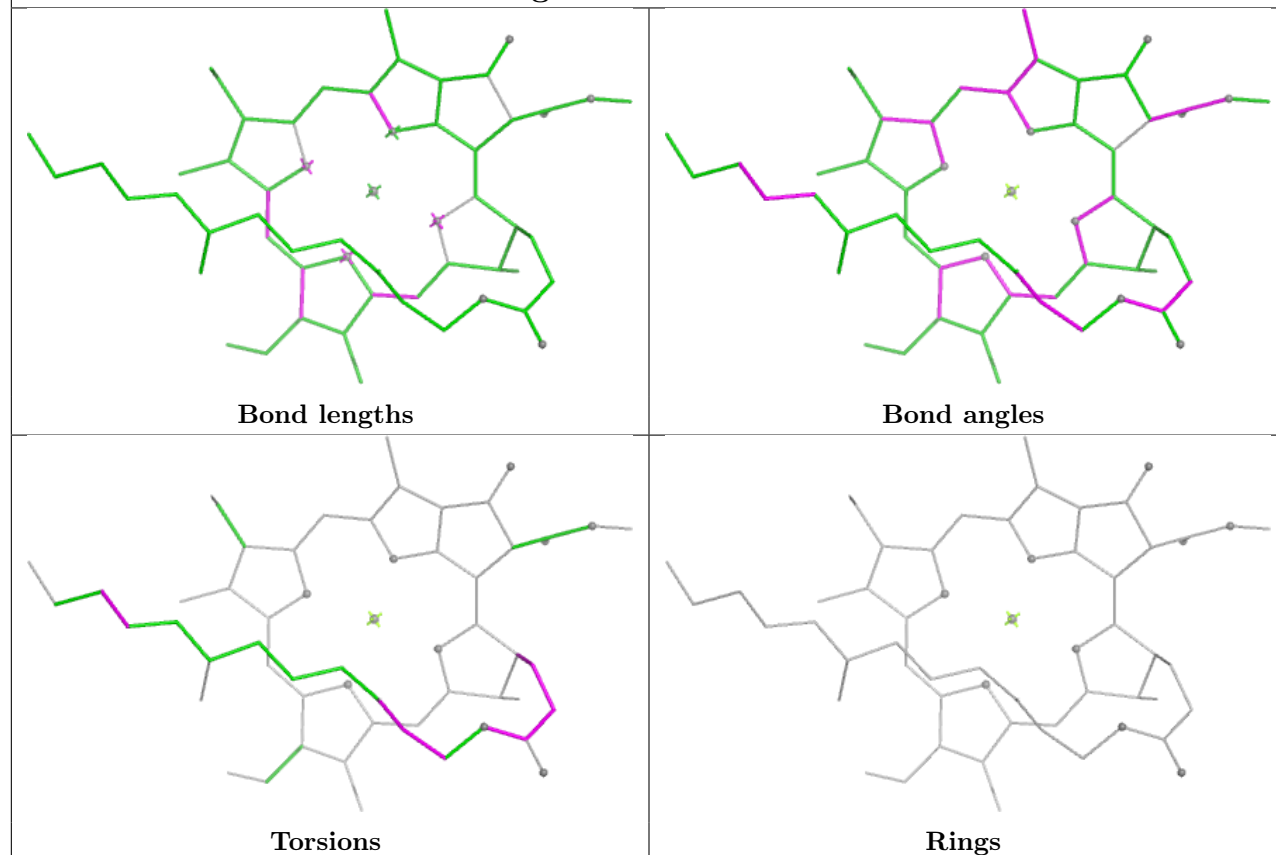


Torsions

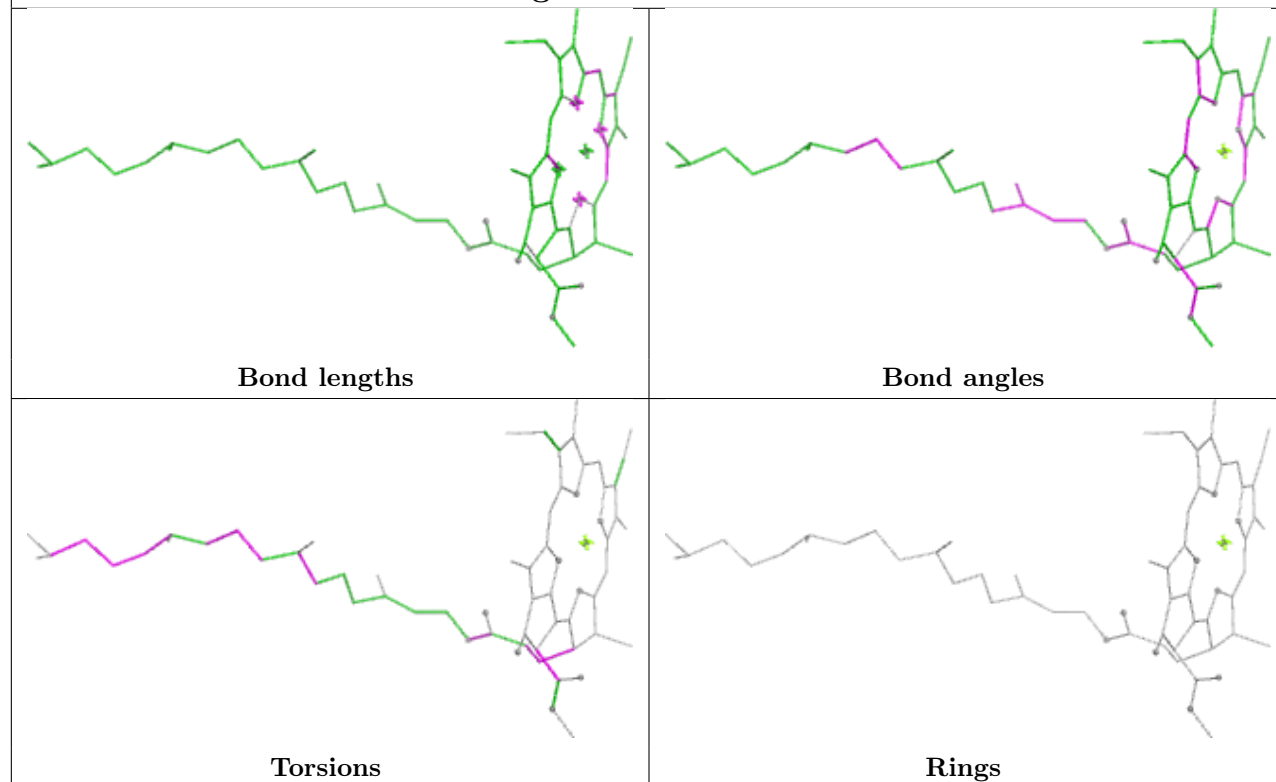


Rings

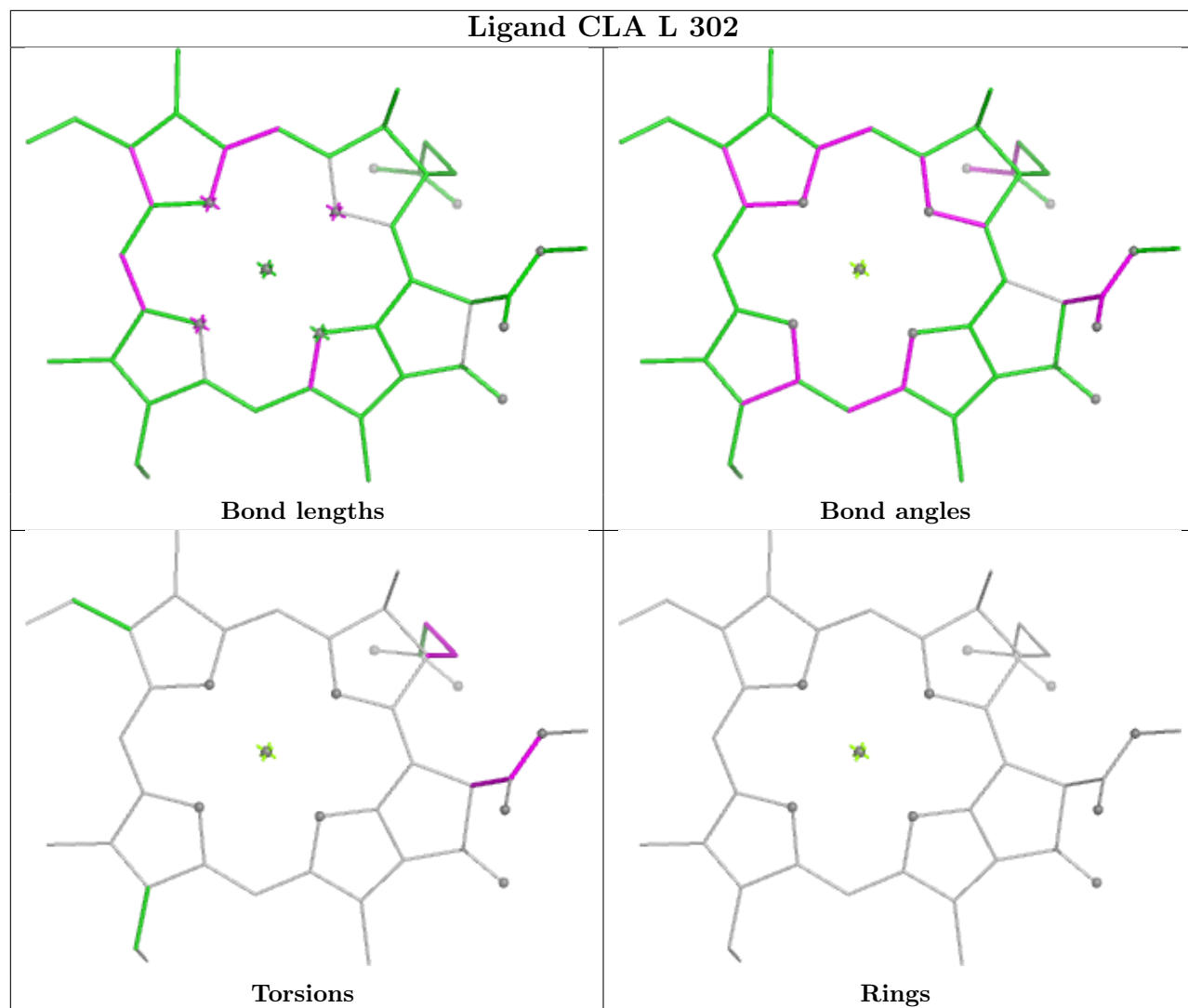
Ligand CLA A 818



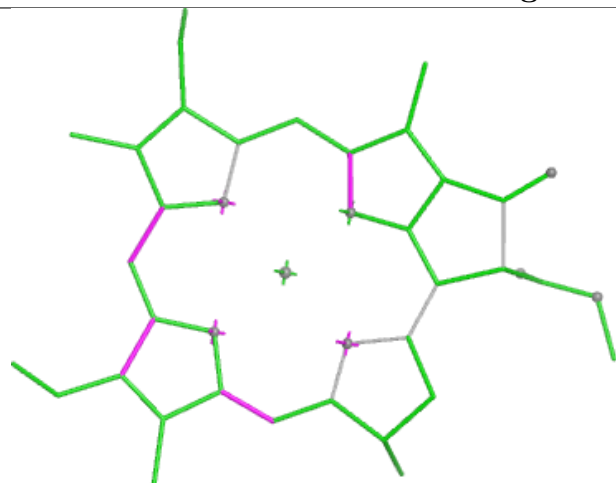
Ligand CLA B 827



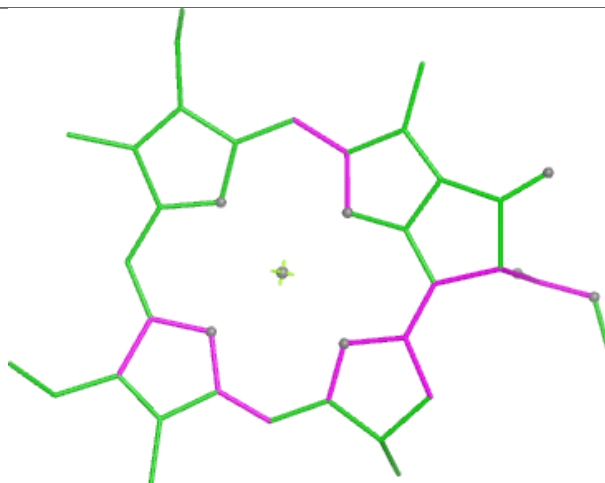
Ligand CLA L 302



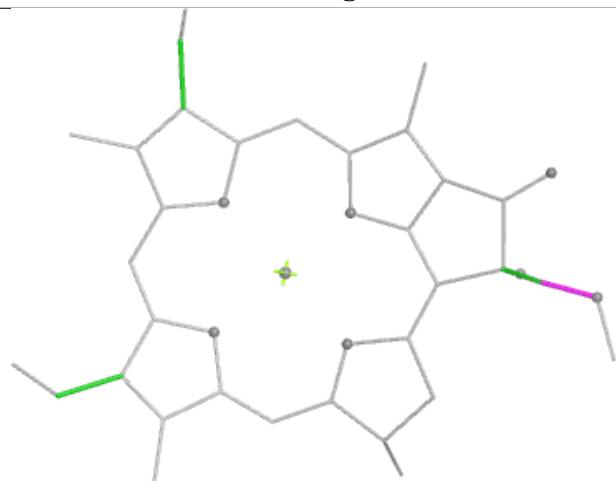
Ligand CLA 1 605



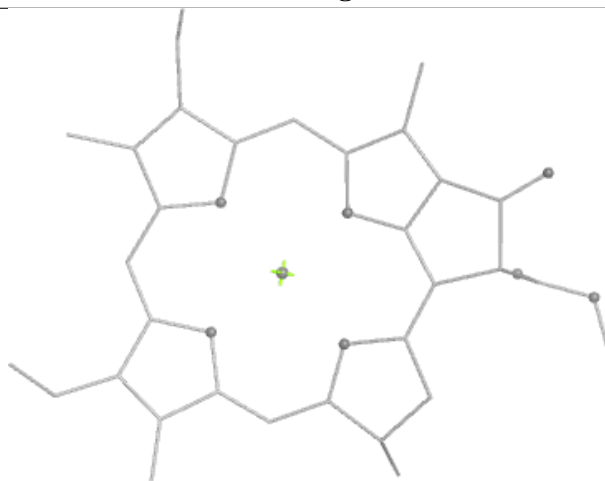
Bond lengths



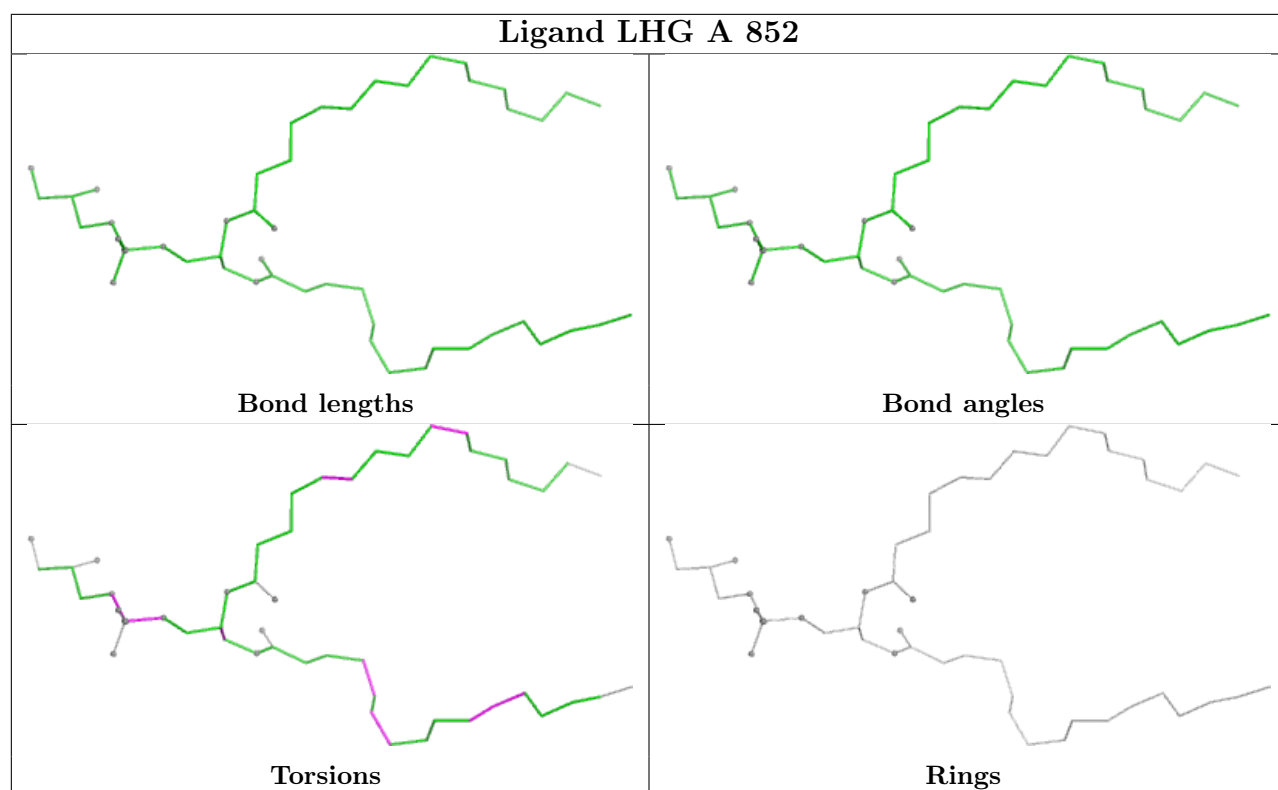
Bond angles



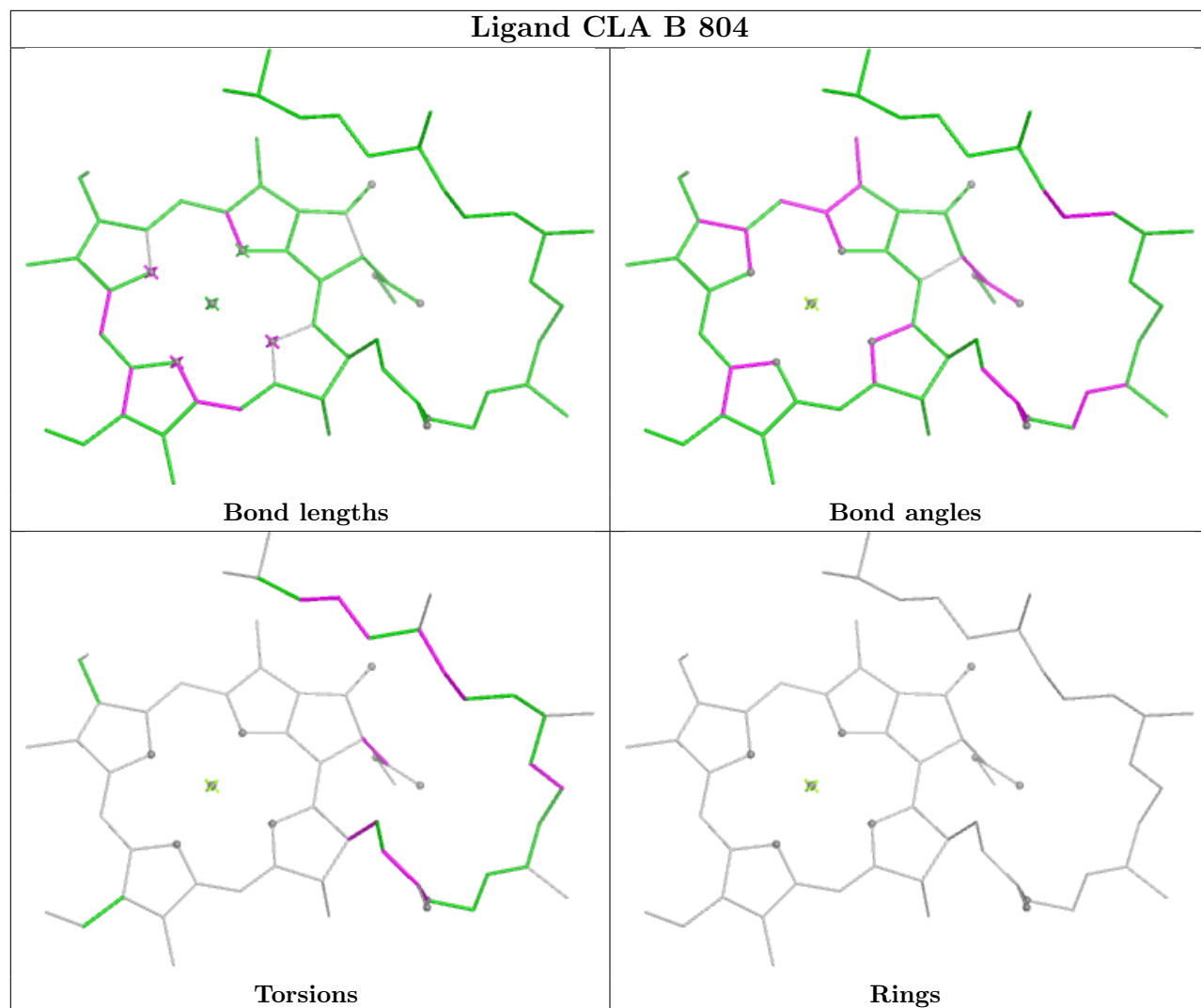
Torsions



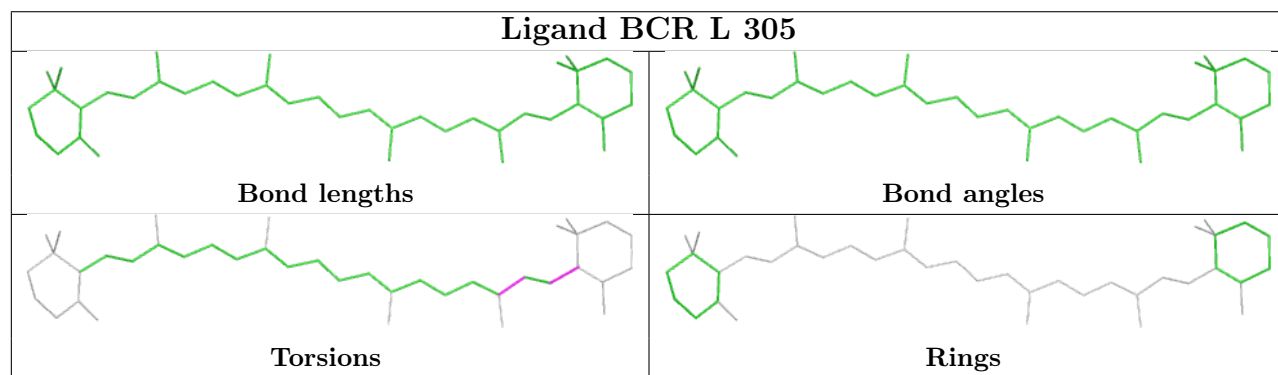
Rings



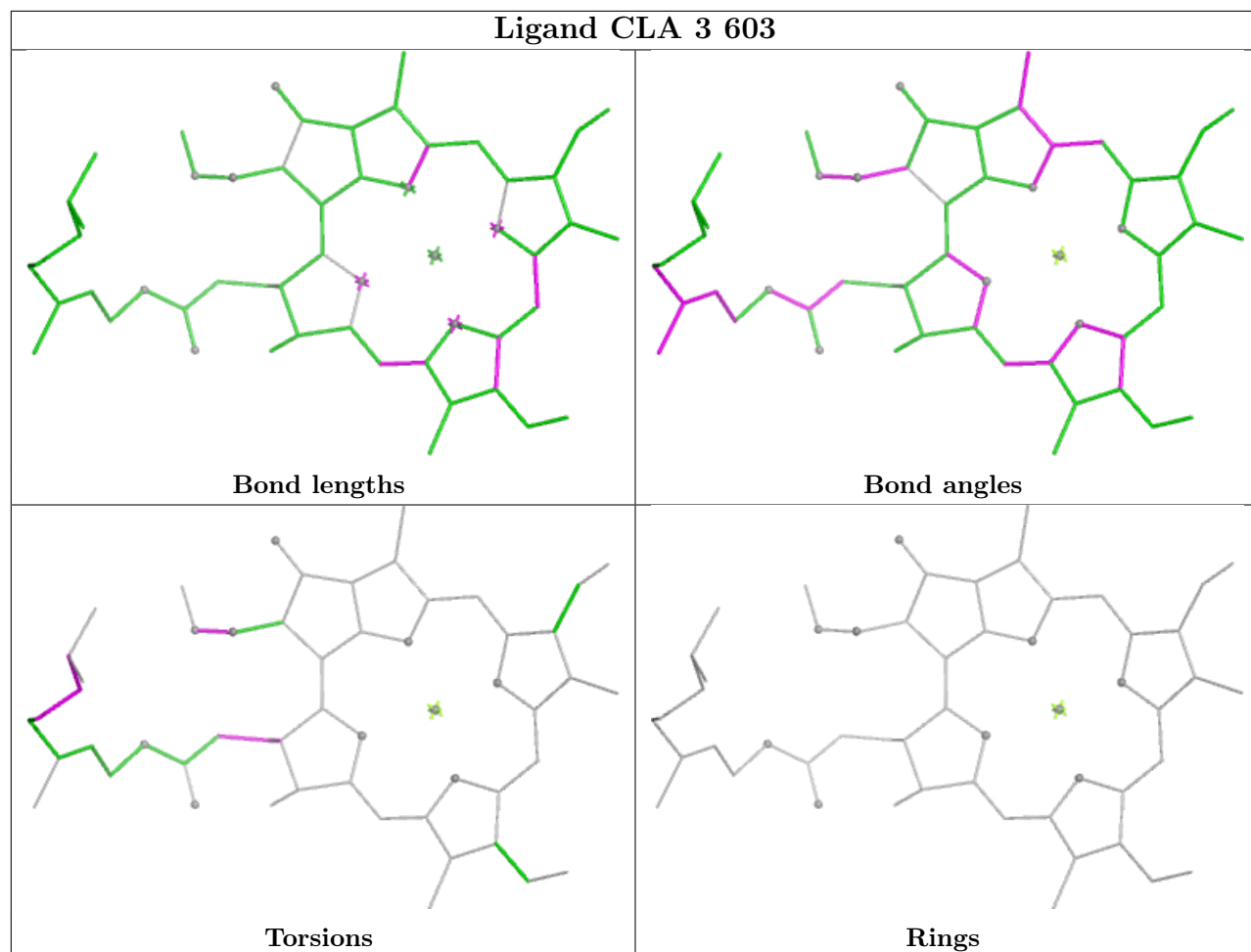
Ligand CLA B 804



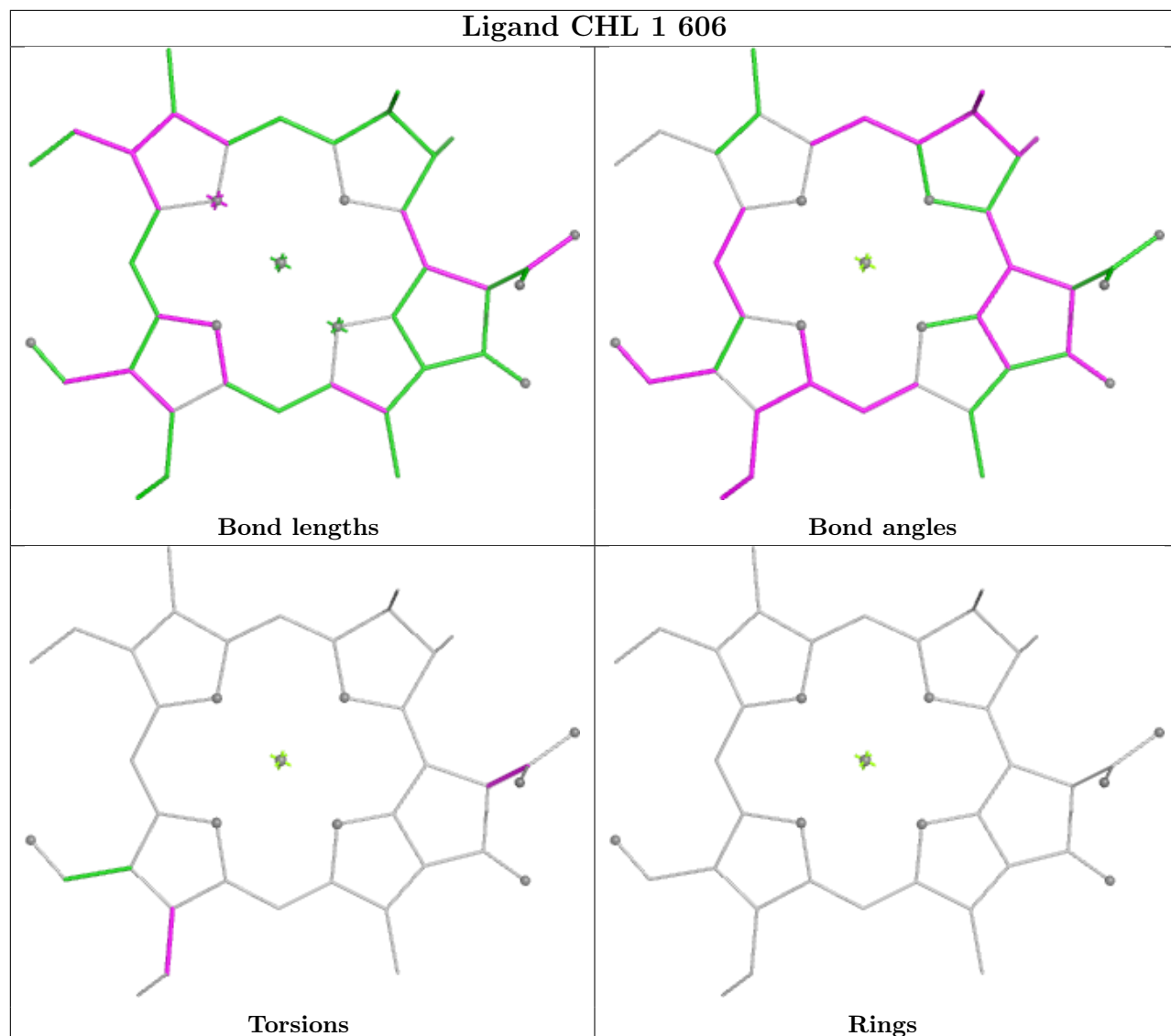
Ligand BCR L 305

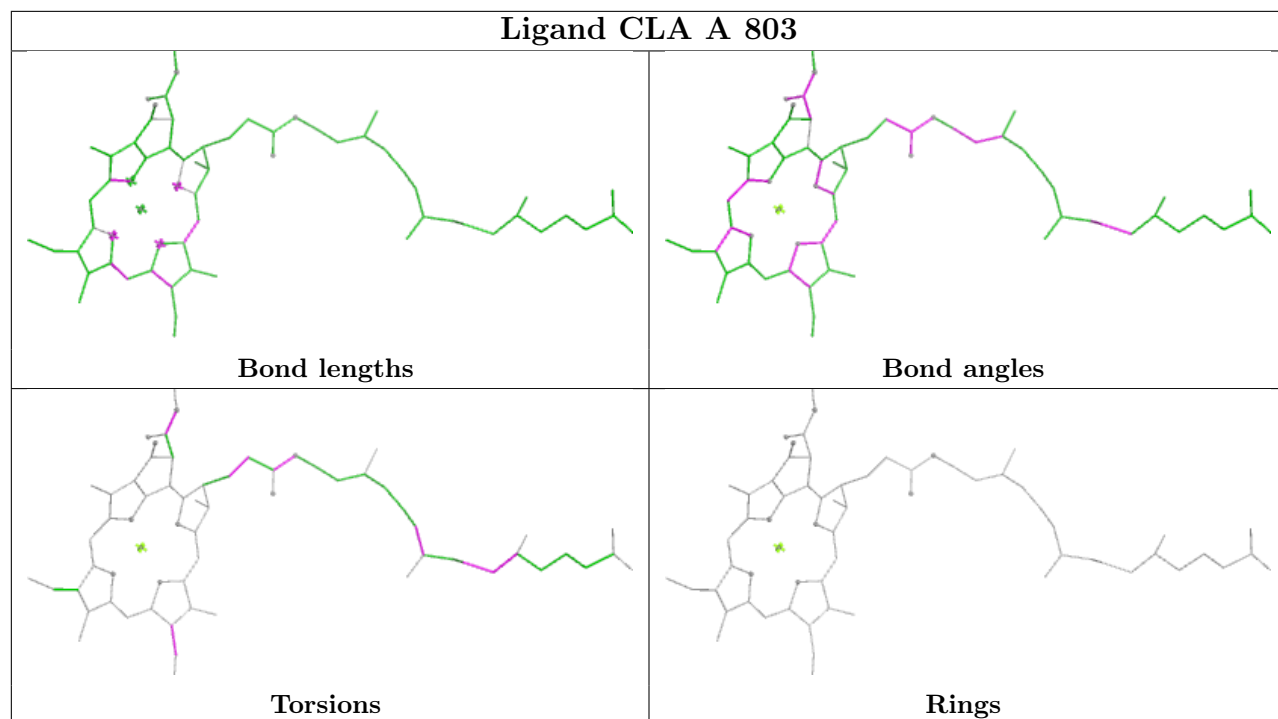


Ligand CLA 3 603

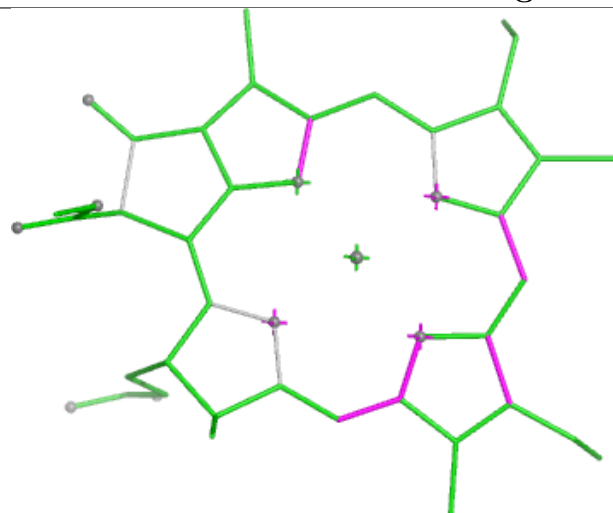


Ligand CHL 1 606

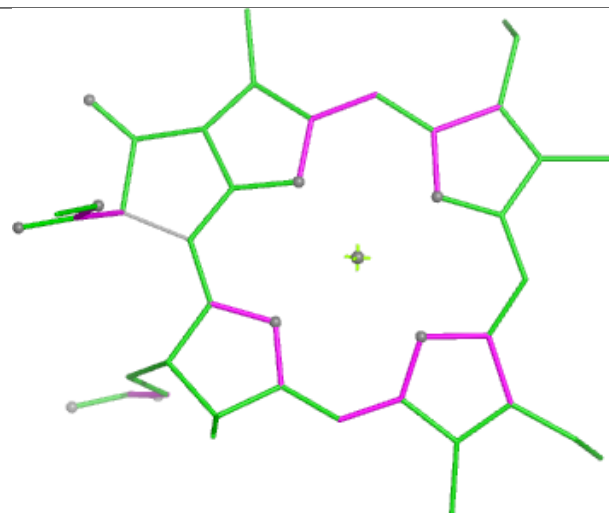




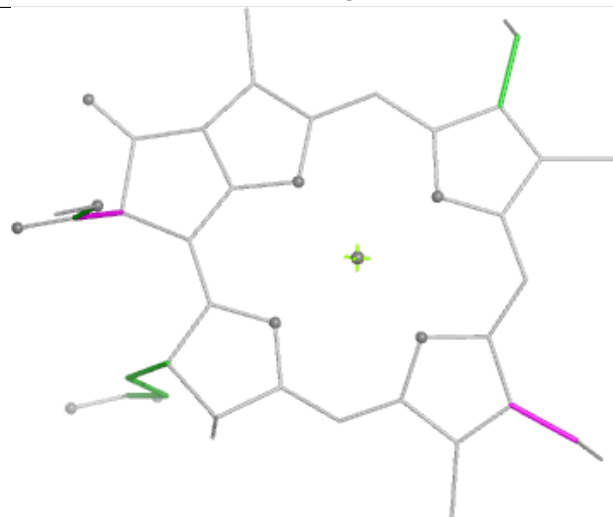
Ligand CLA A 820



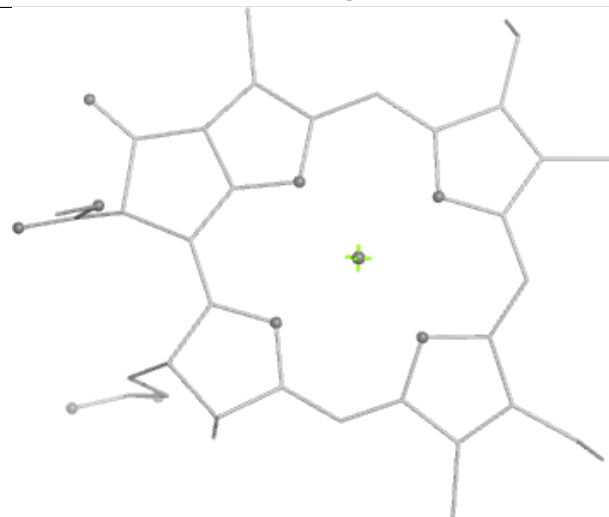
Bond lengths



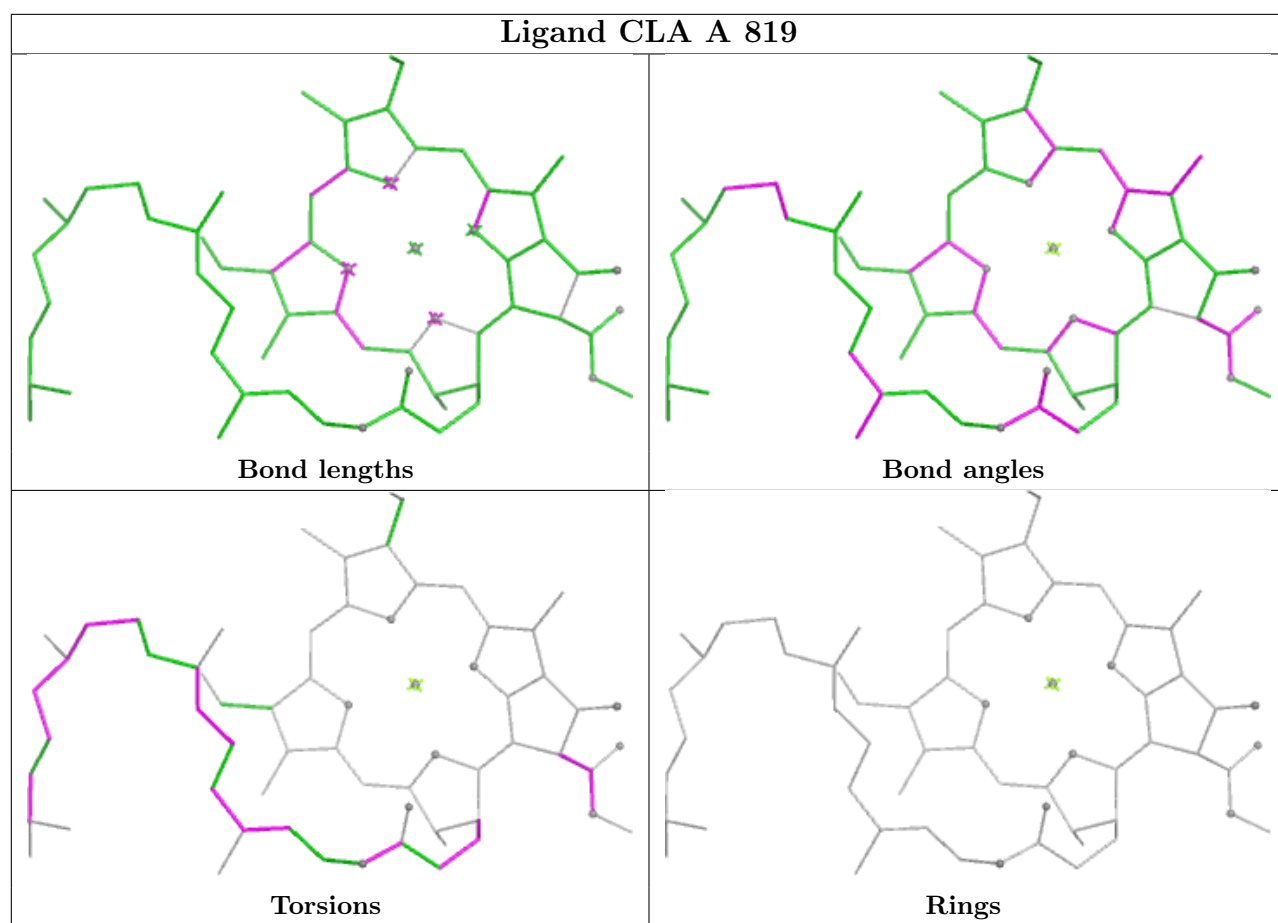
Bond angles



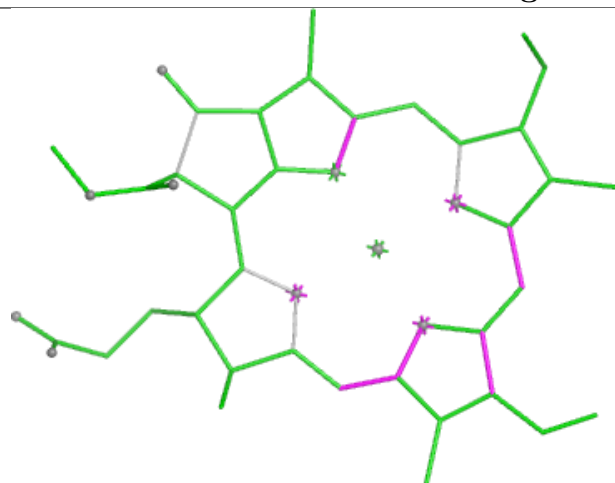
Torsions



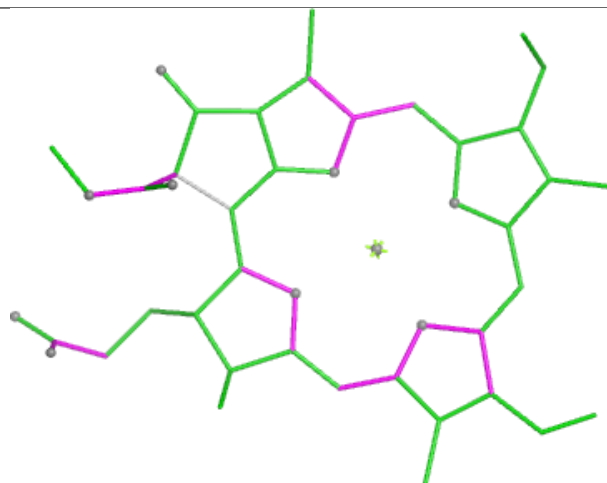
Rings



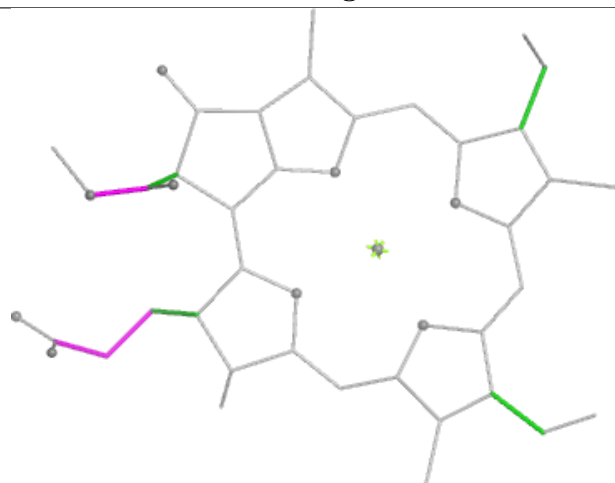
Ligand CLA 1 611



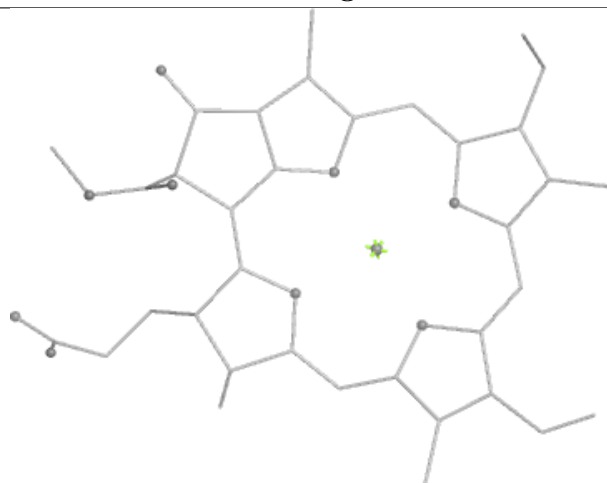
Bond lengths



Bond angles

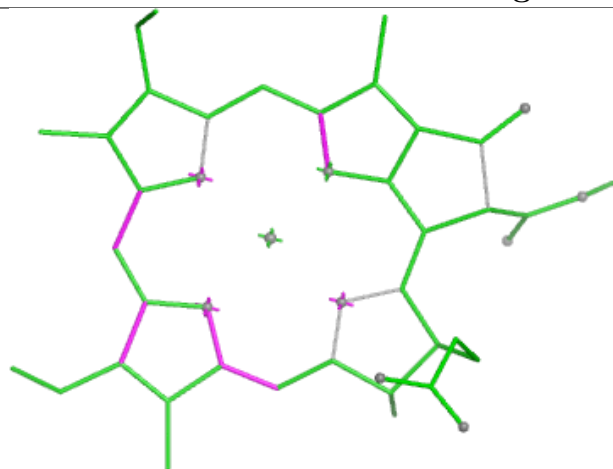


Torsions

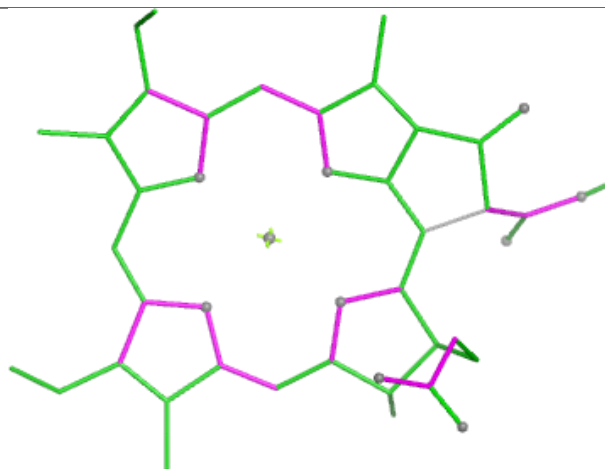


Rings

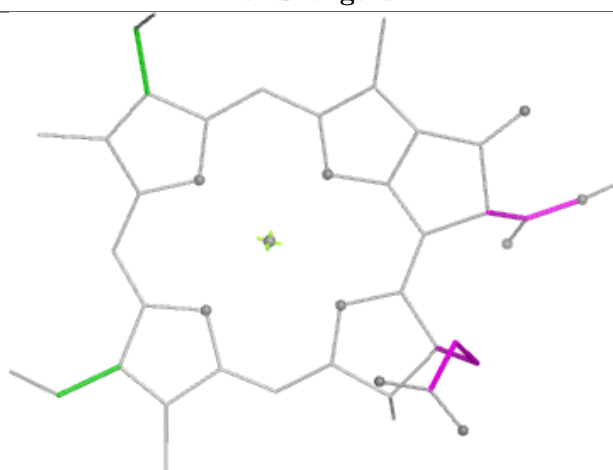
Ligand CLA G 202



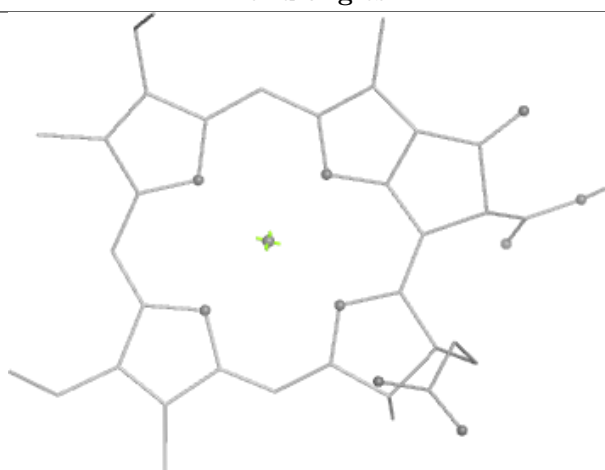
Bond lengths



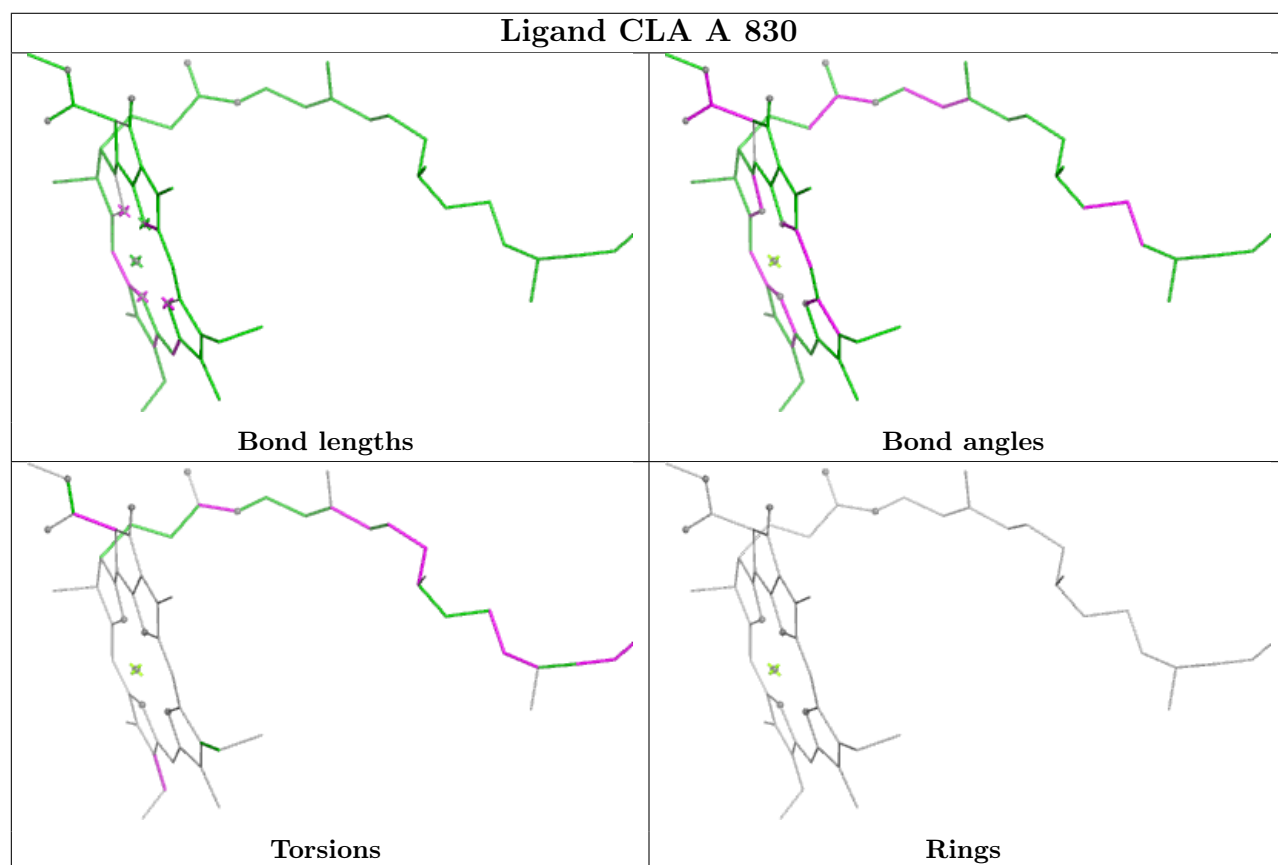
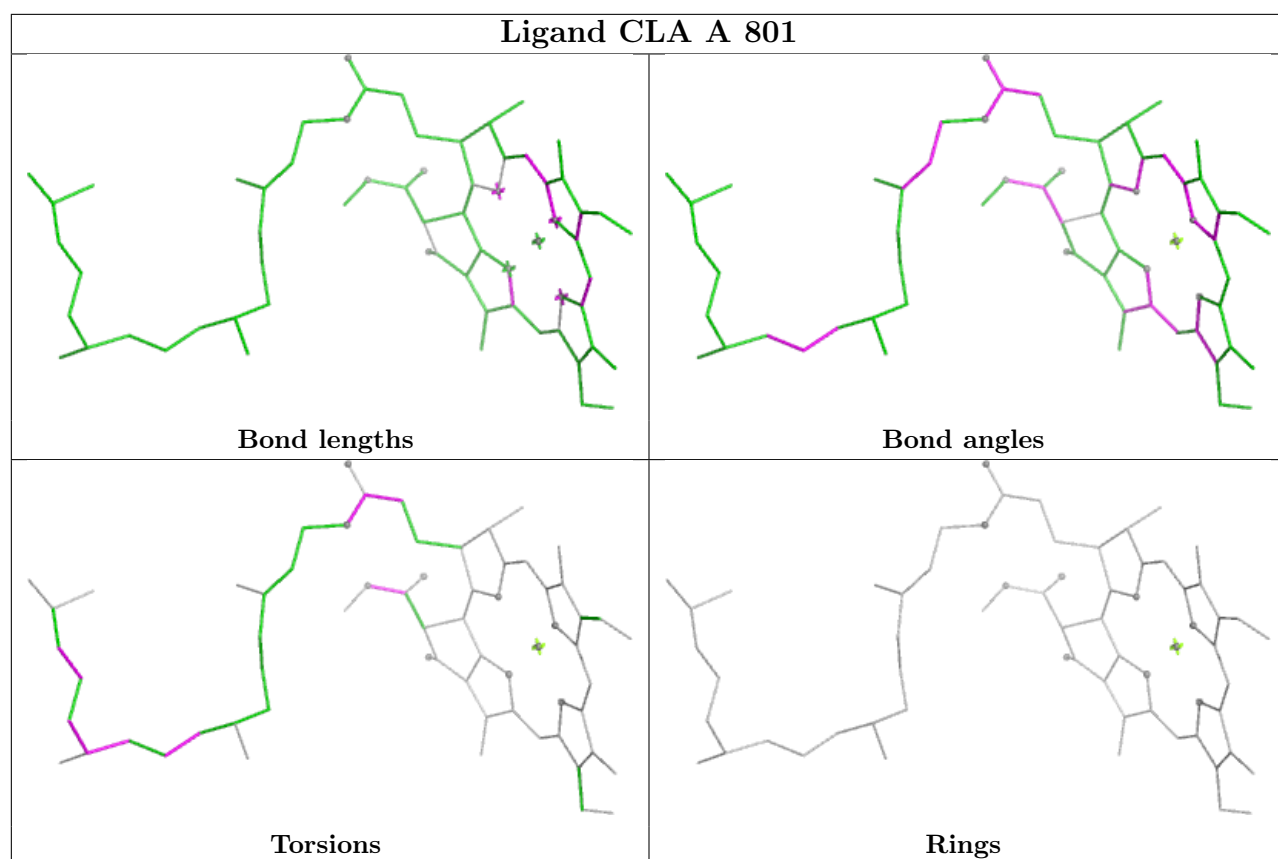
Bond angles

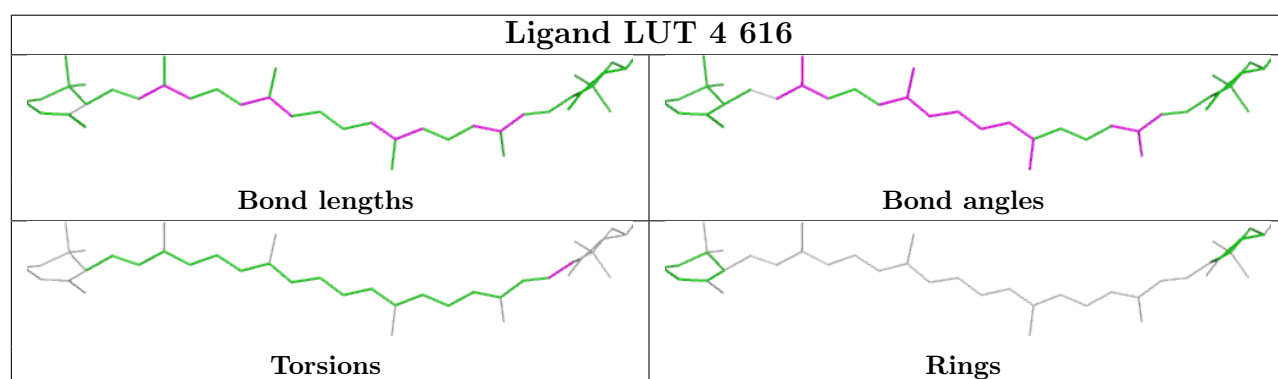
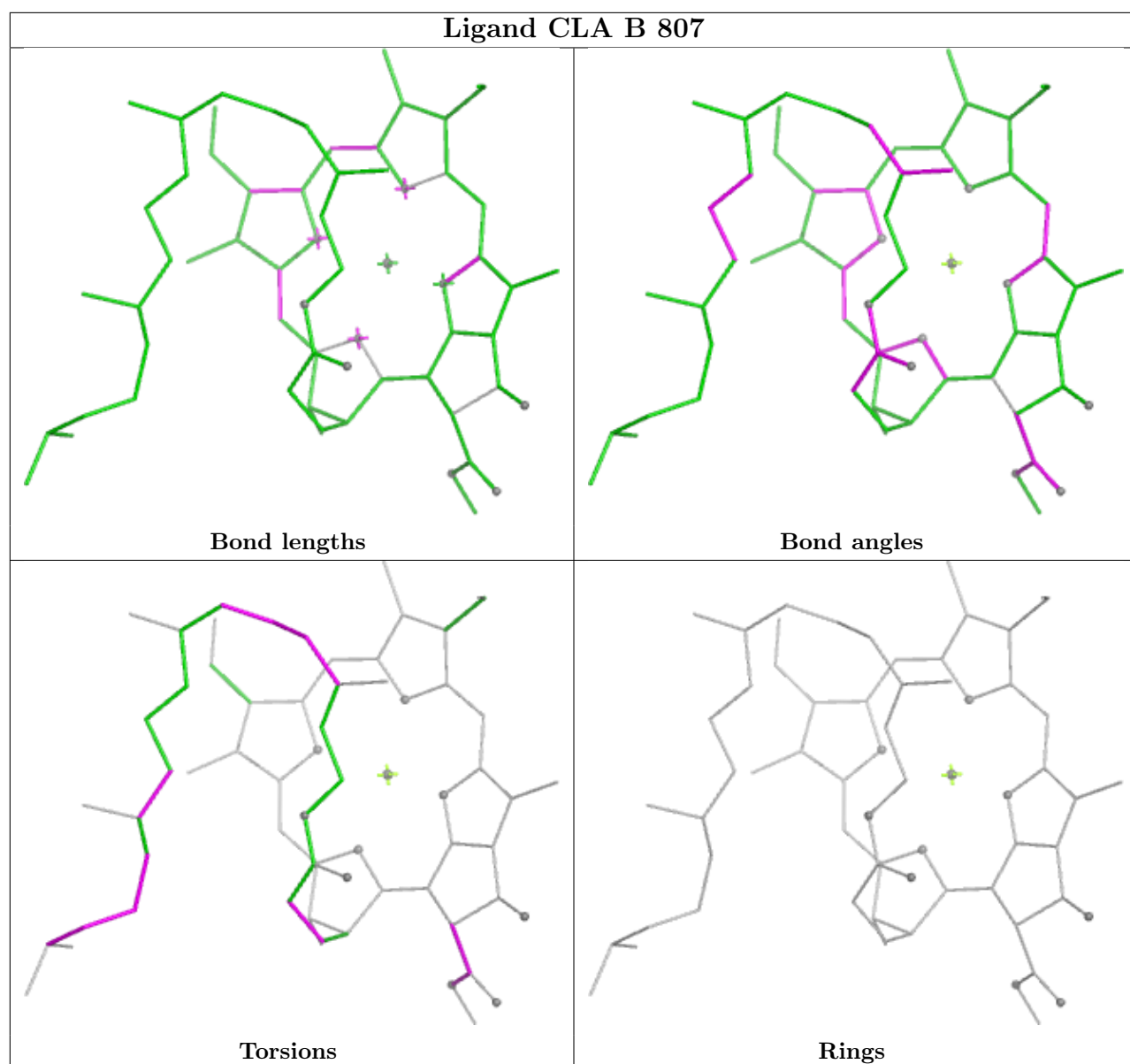


Torsions

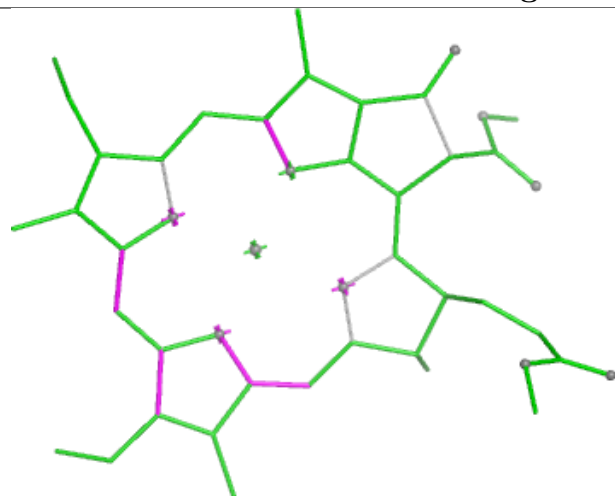


Rings

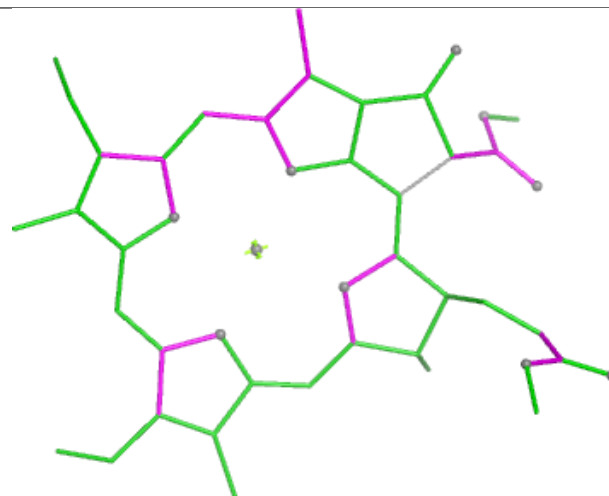




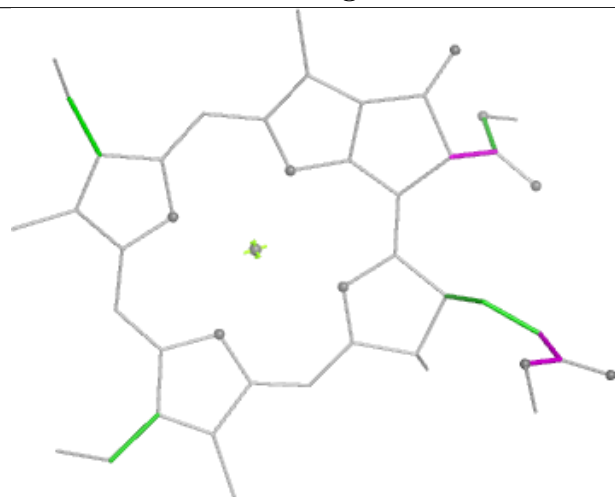
Ligand CLA 4 601



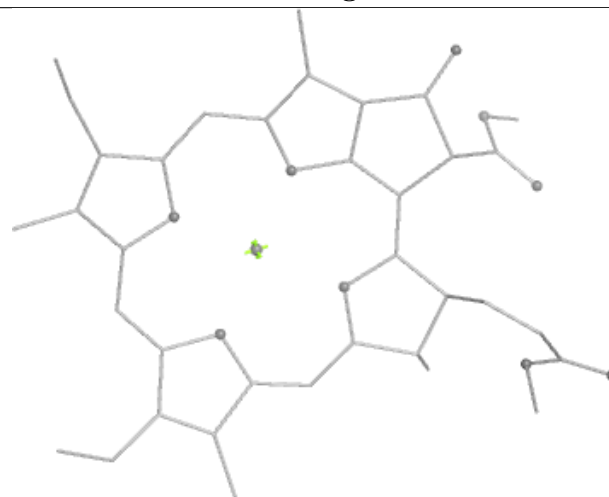
Bond lengths



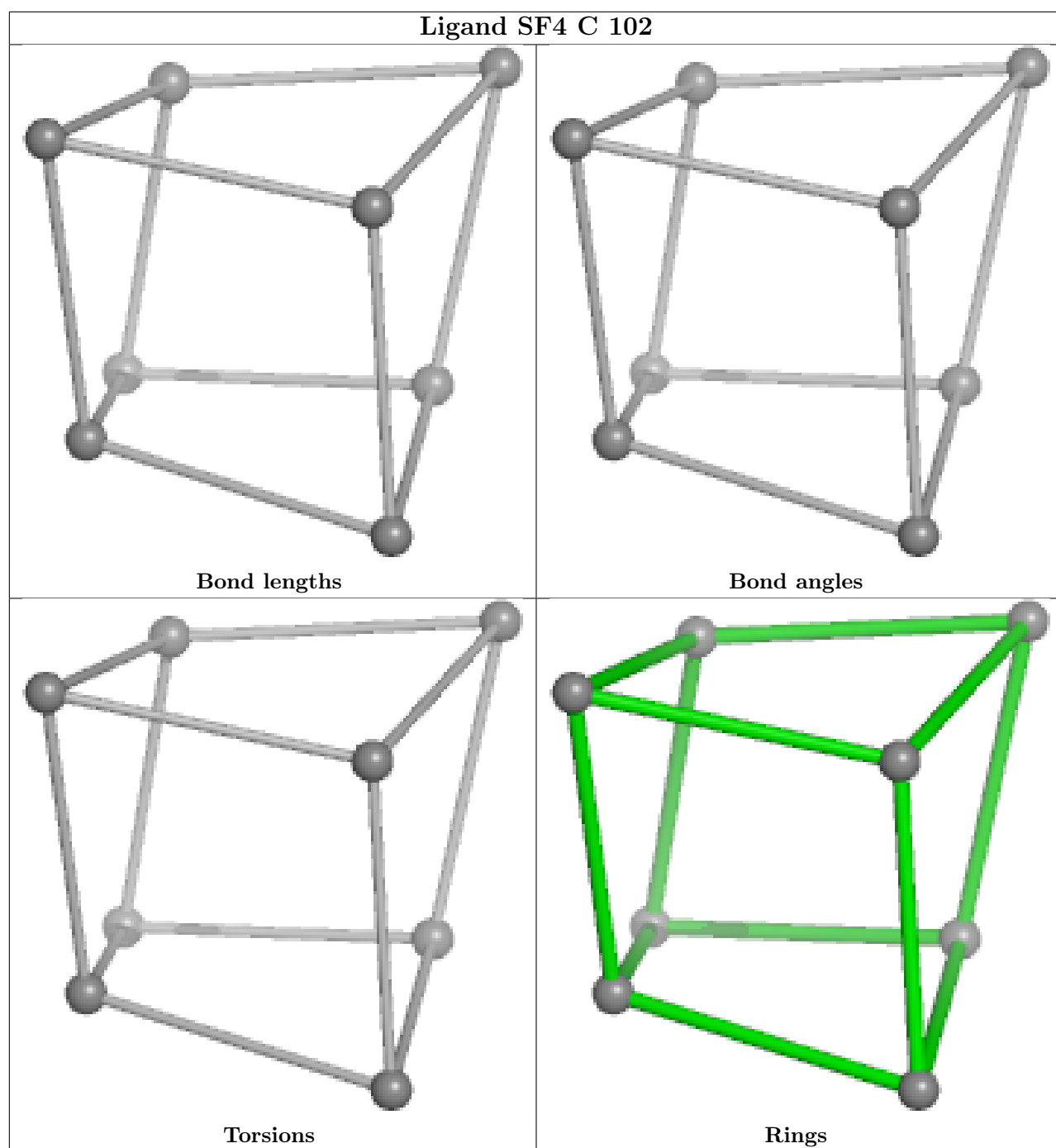
Bond angles



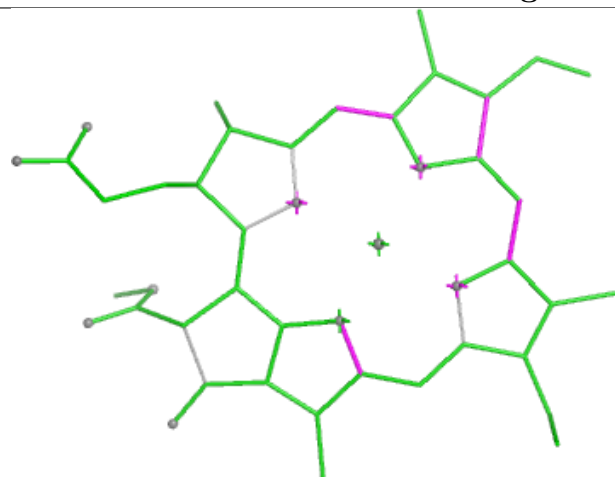
Torsions



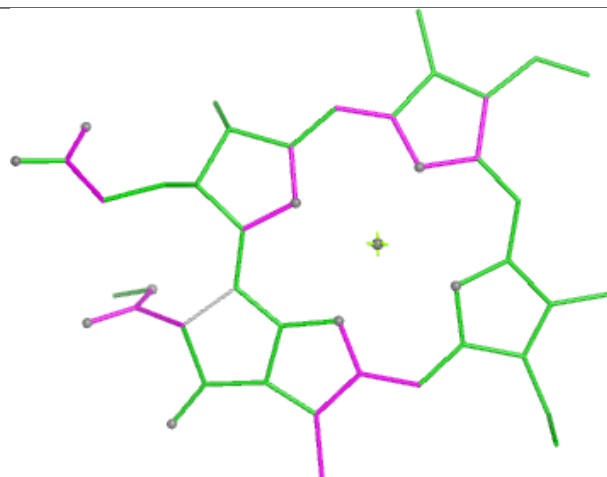
Rings



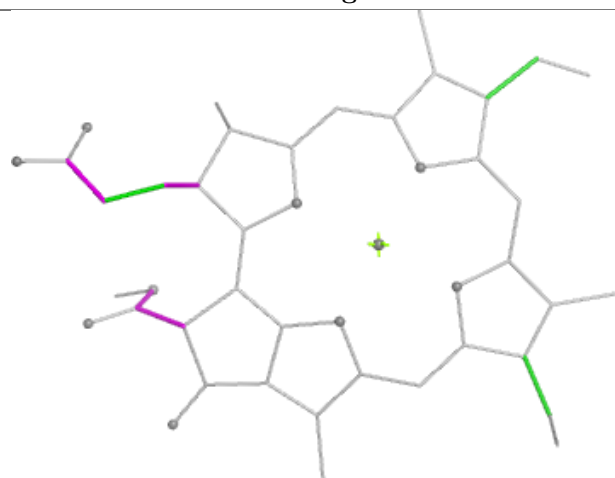
Ligand CLA 4 603



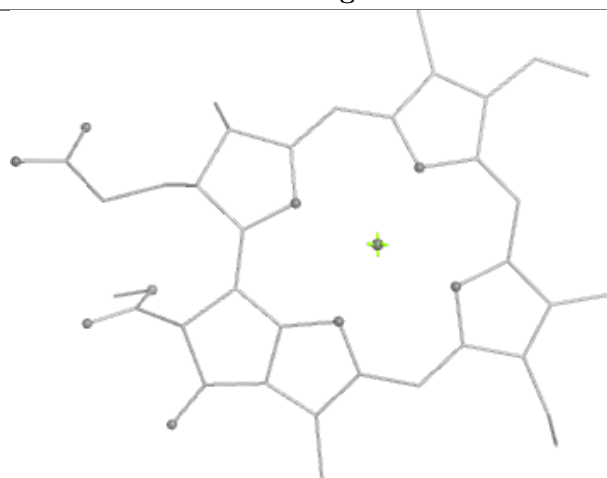
Bond lengths



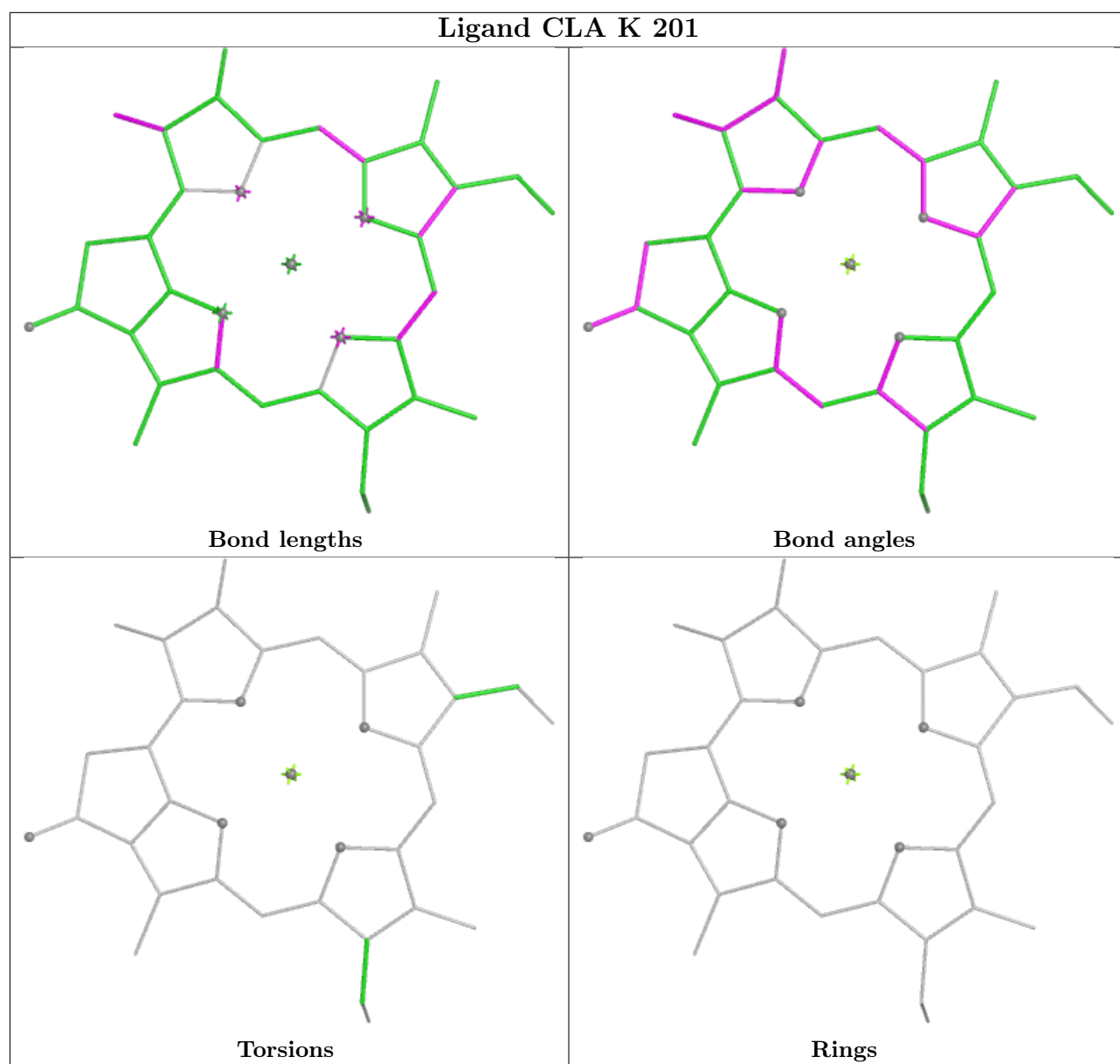
Bond angles



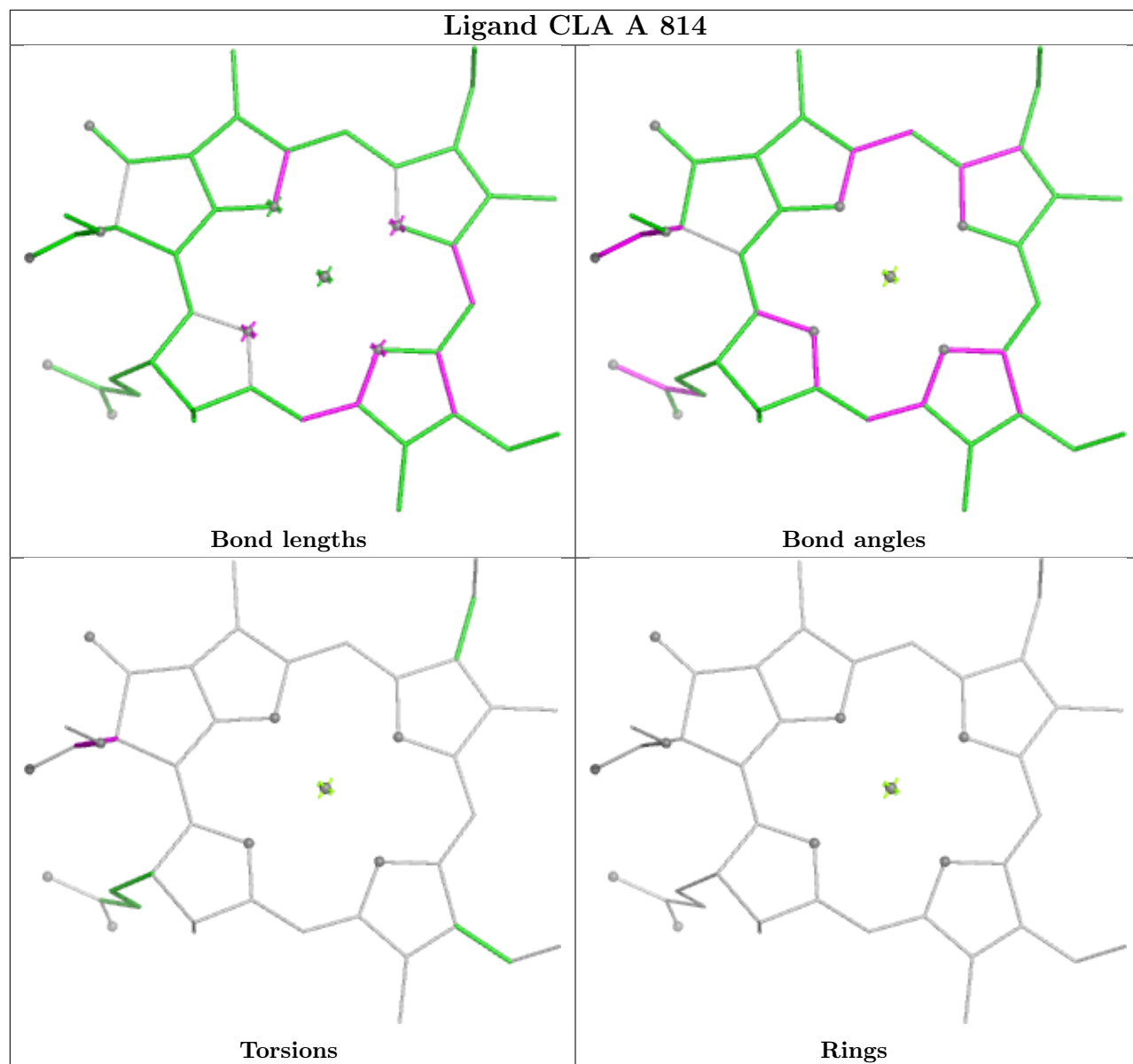
Torsions

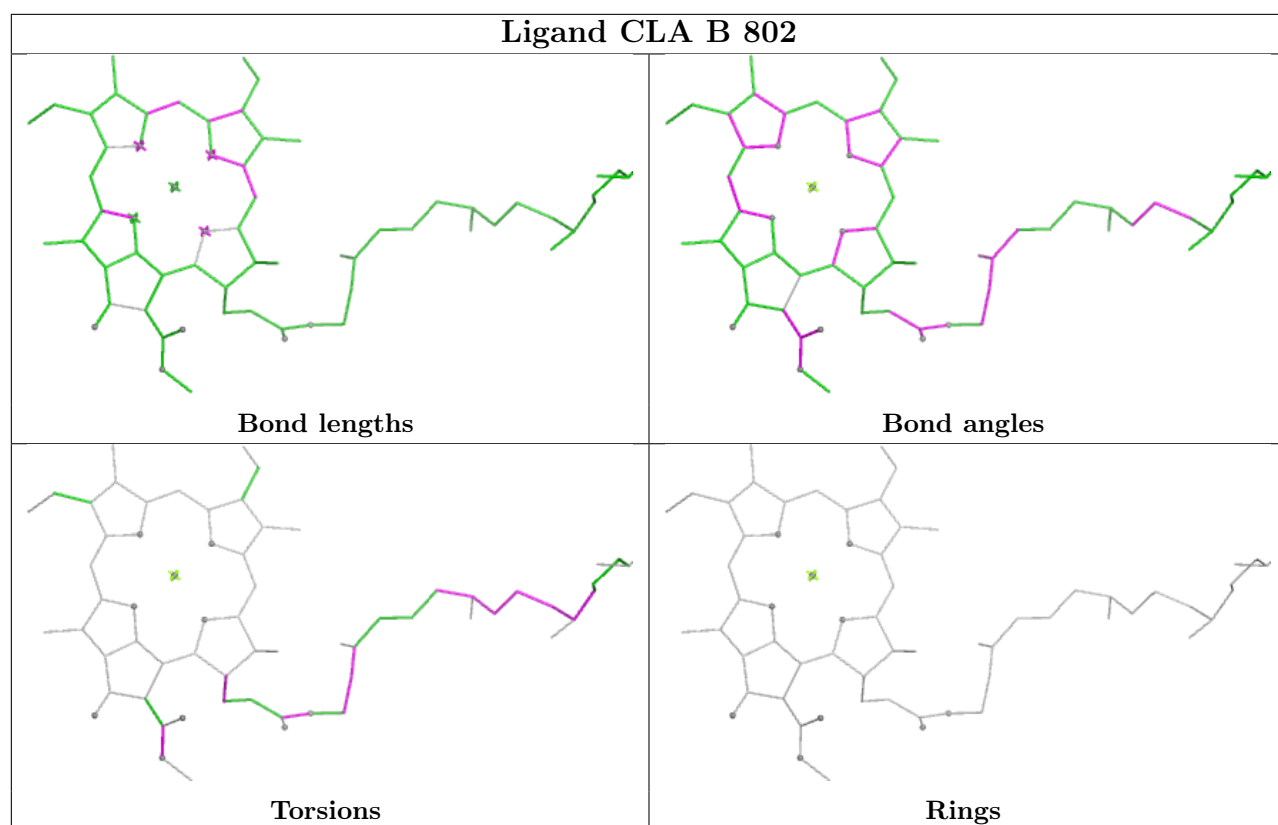


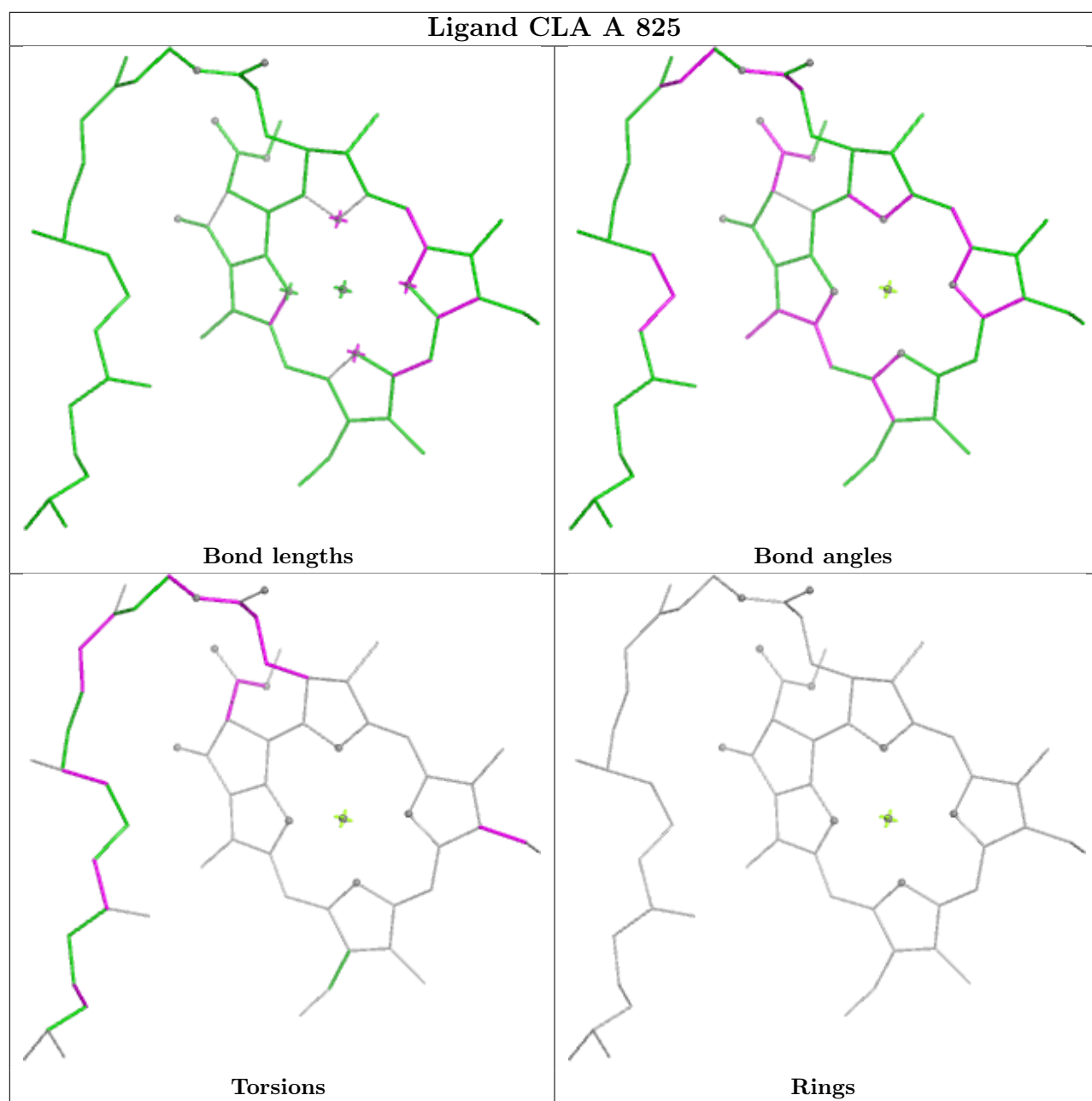
Rings



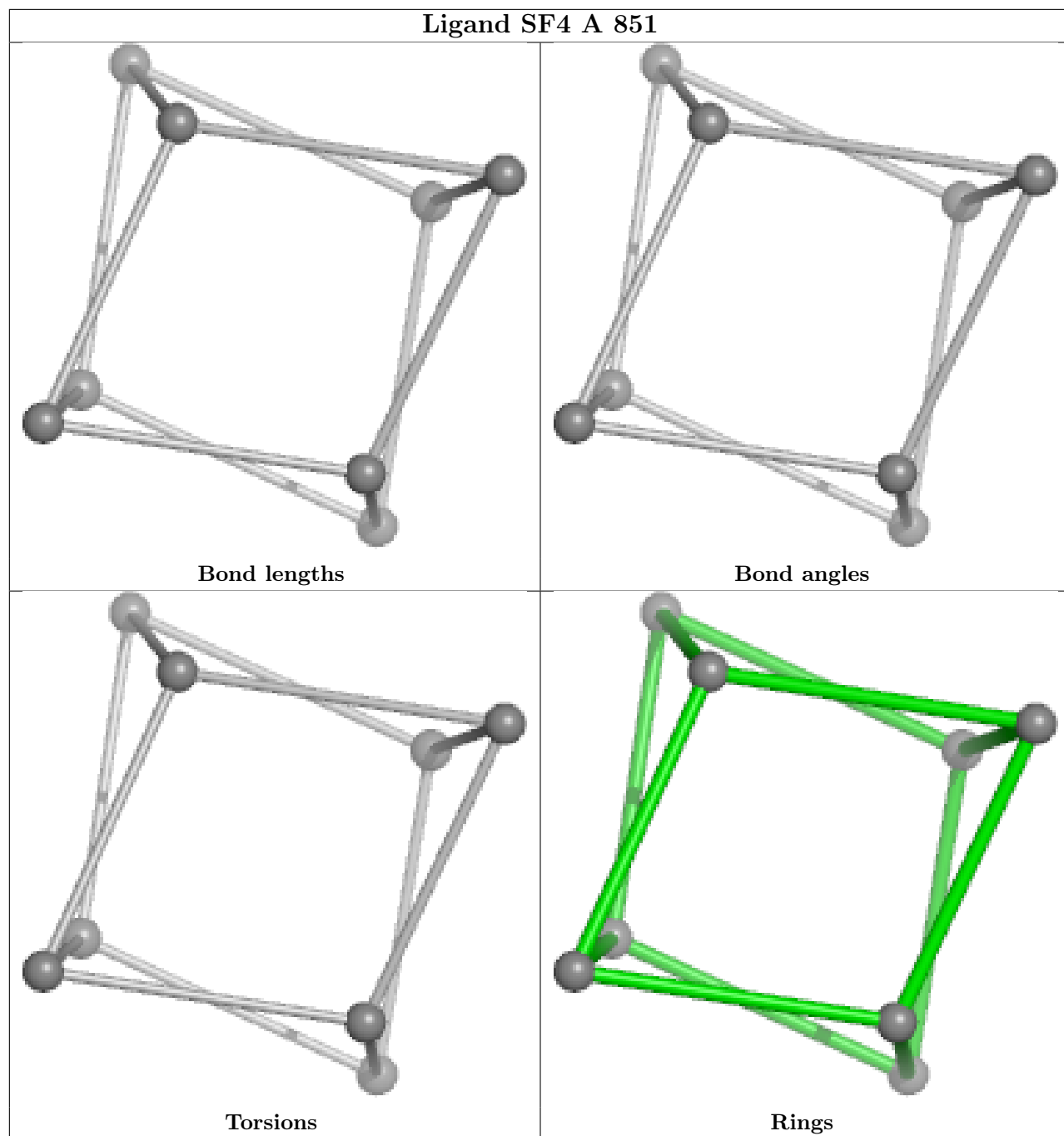
Ligand CLA A 814



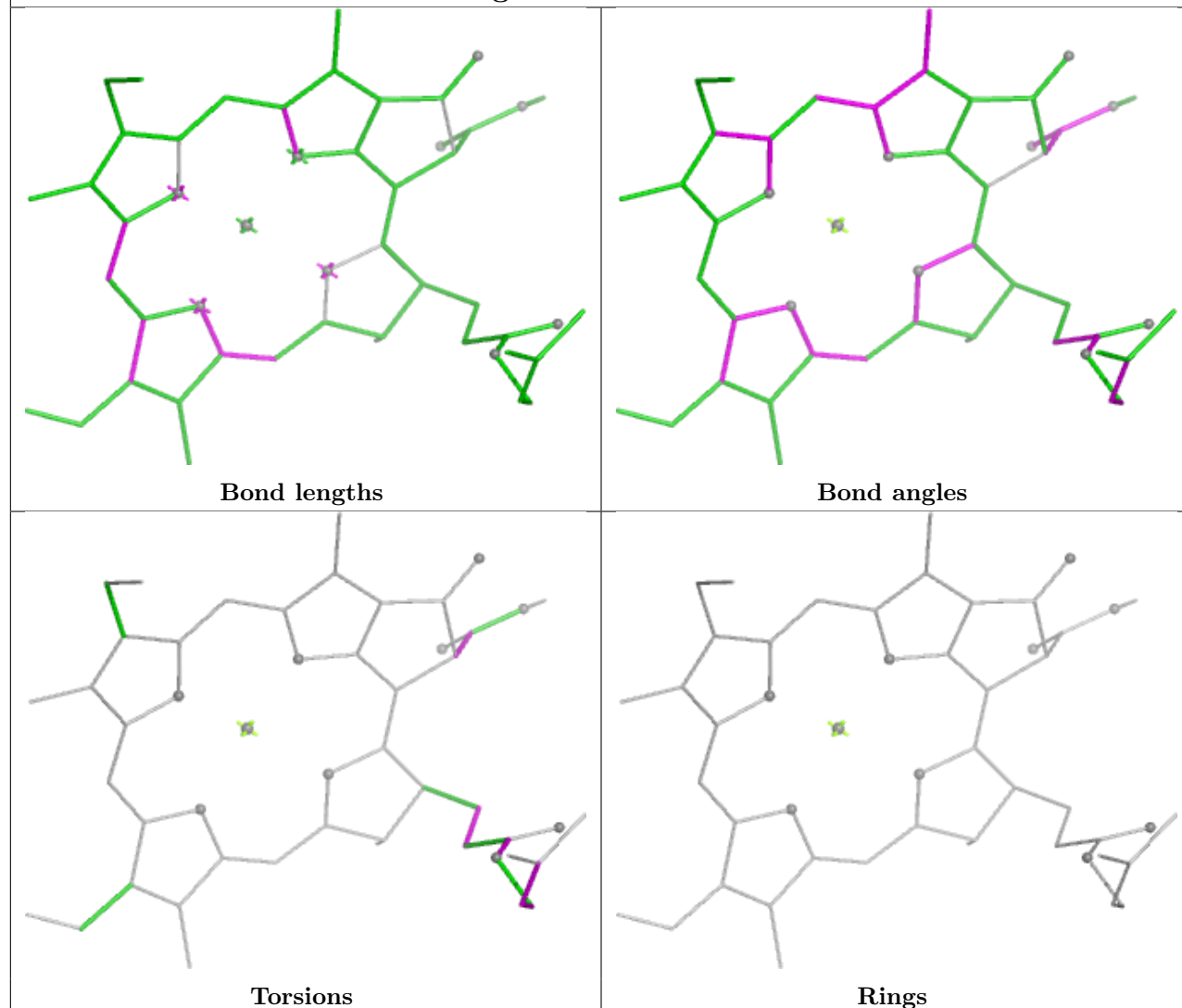




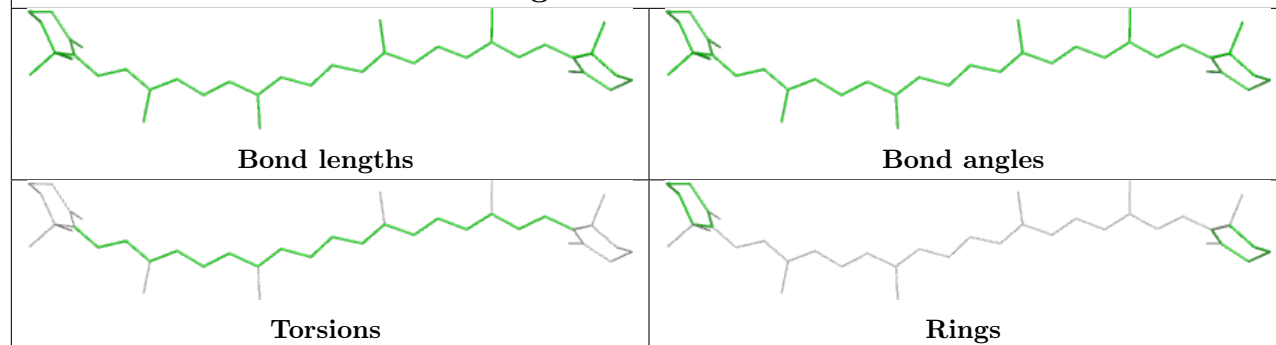
Ligand SF4 A 851

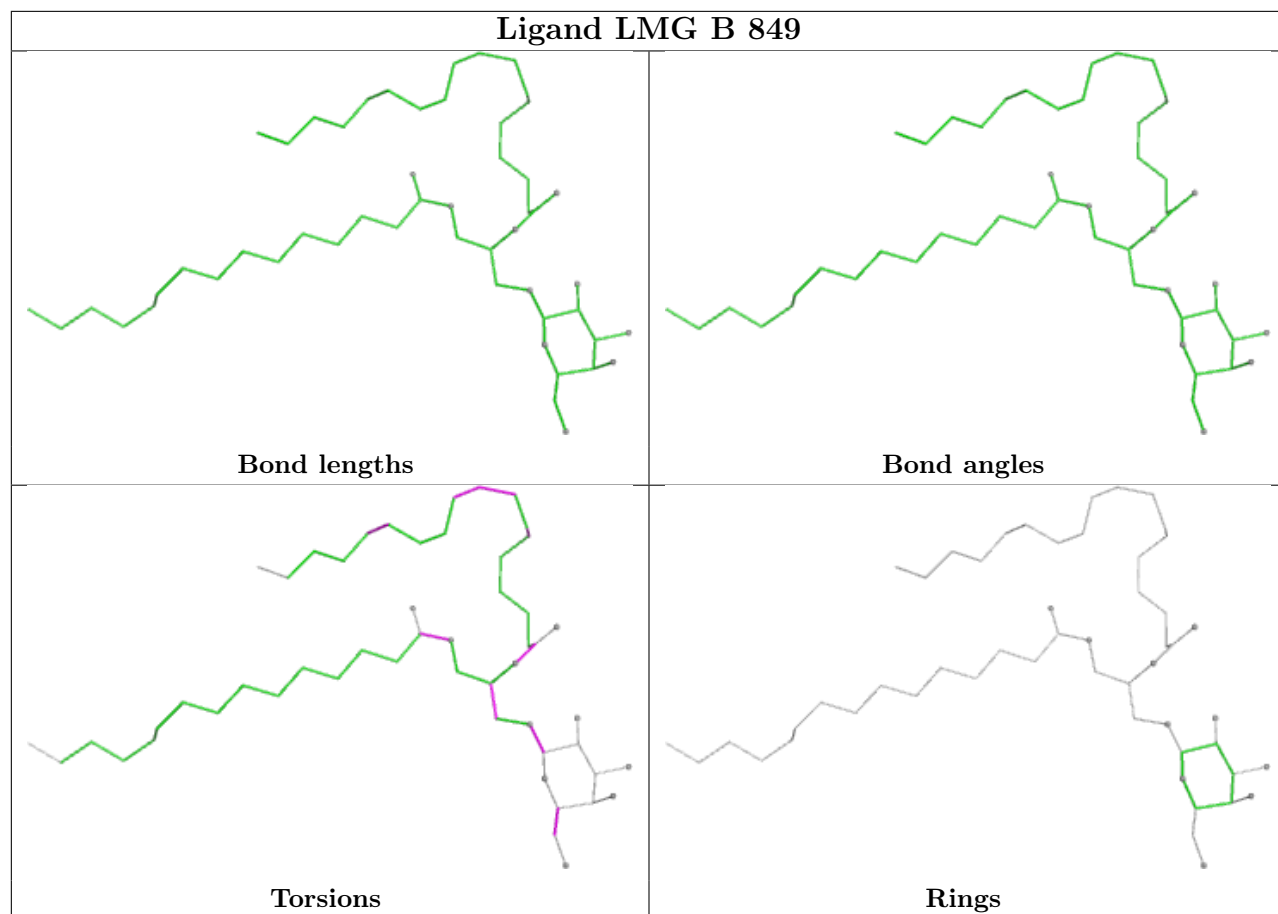


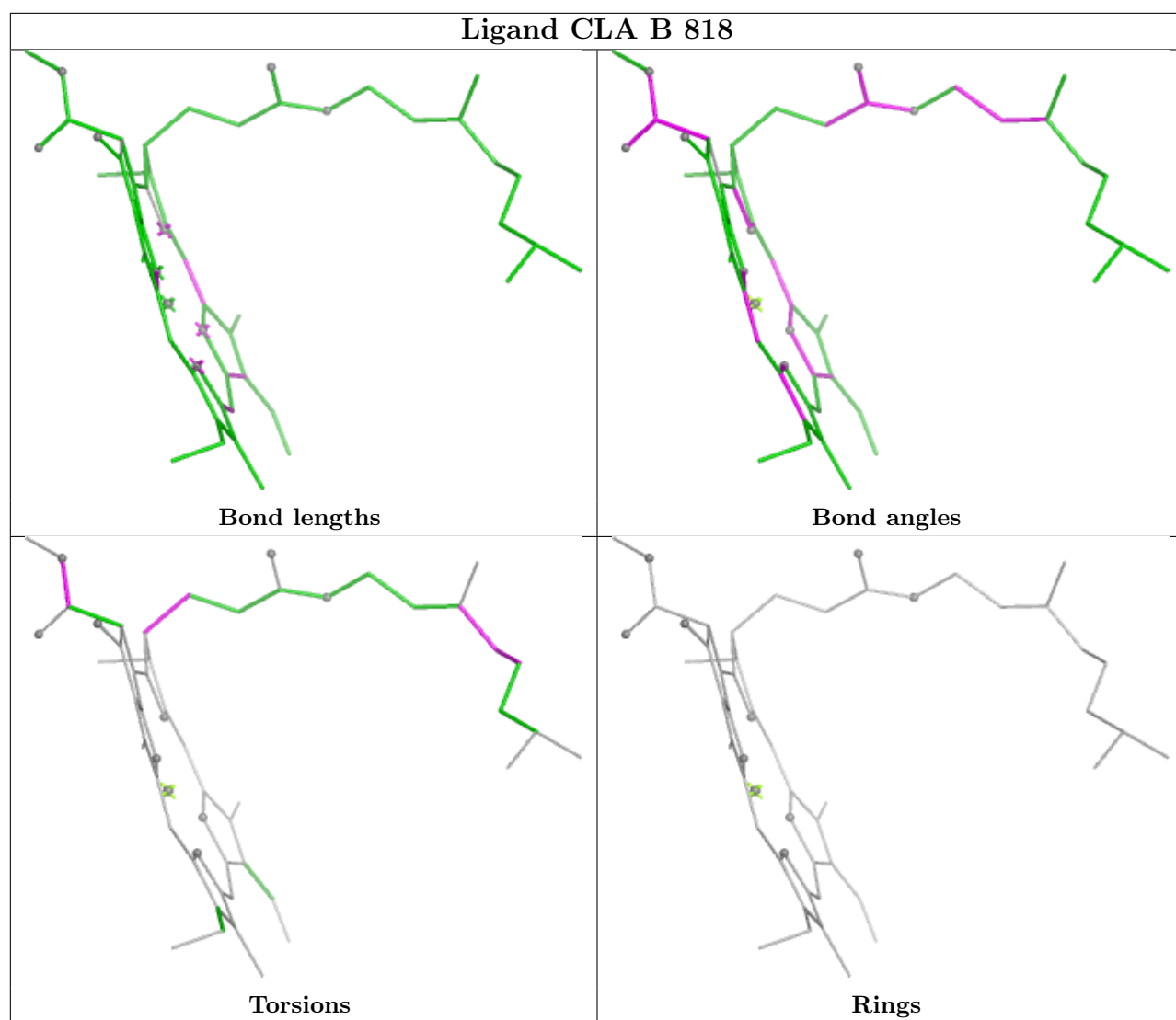
Ligand CLA A 808

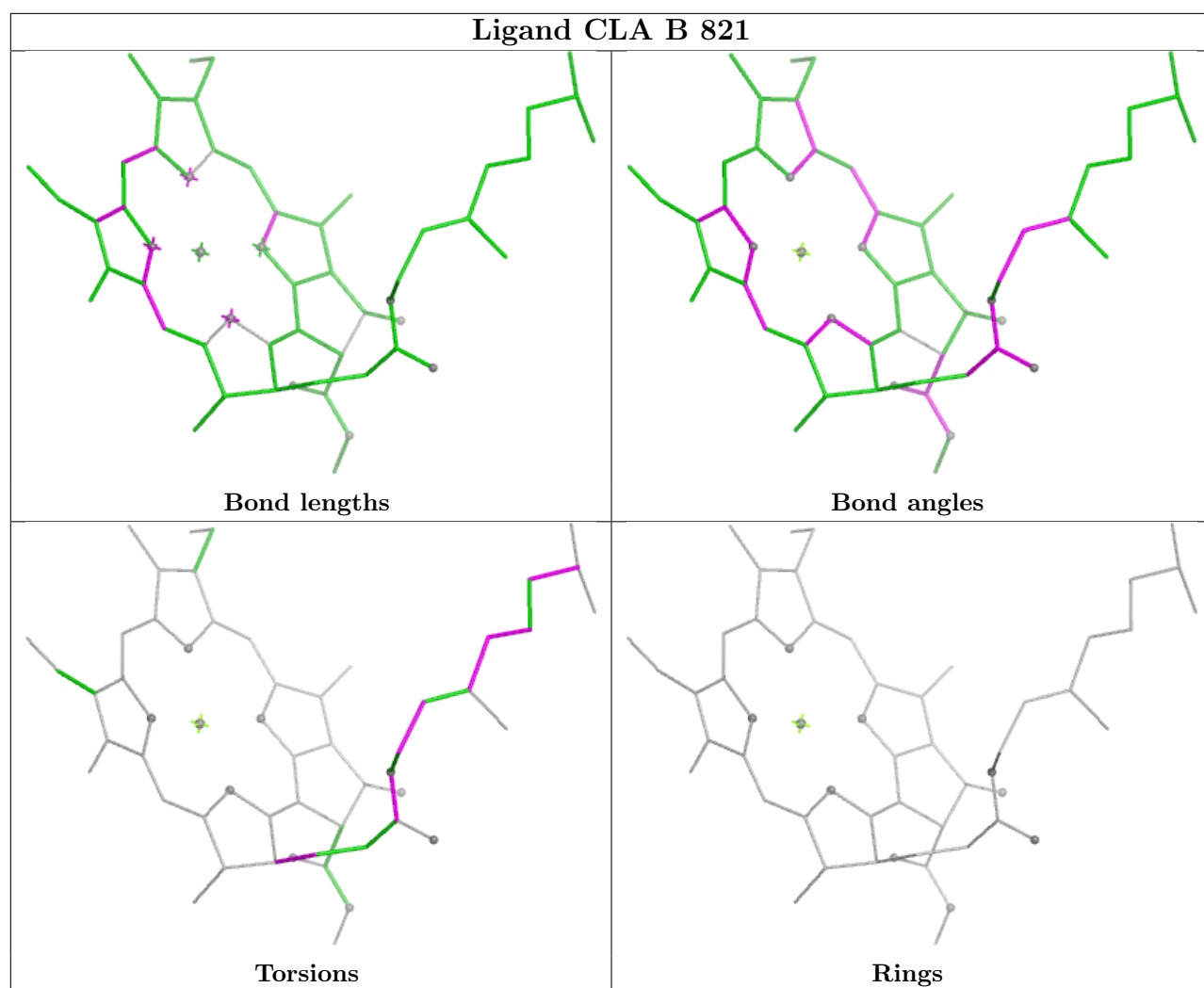


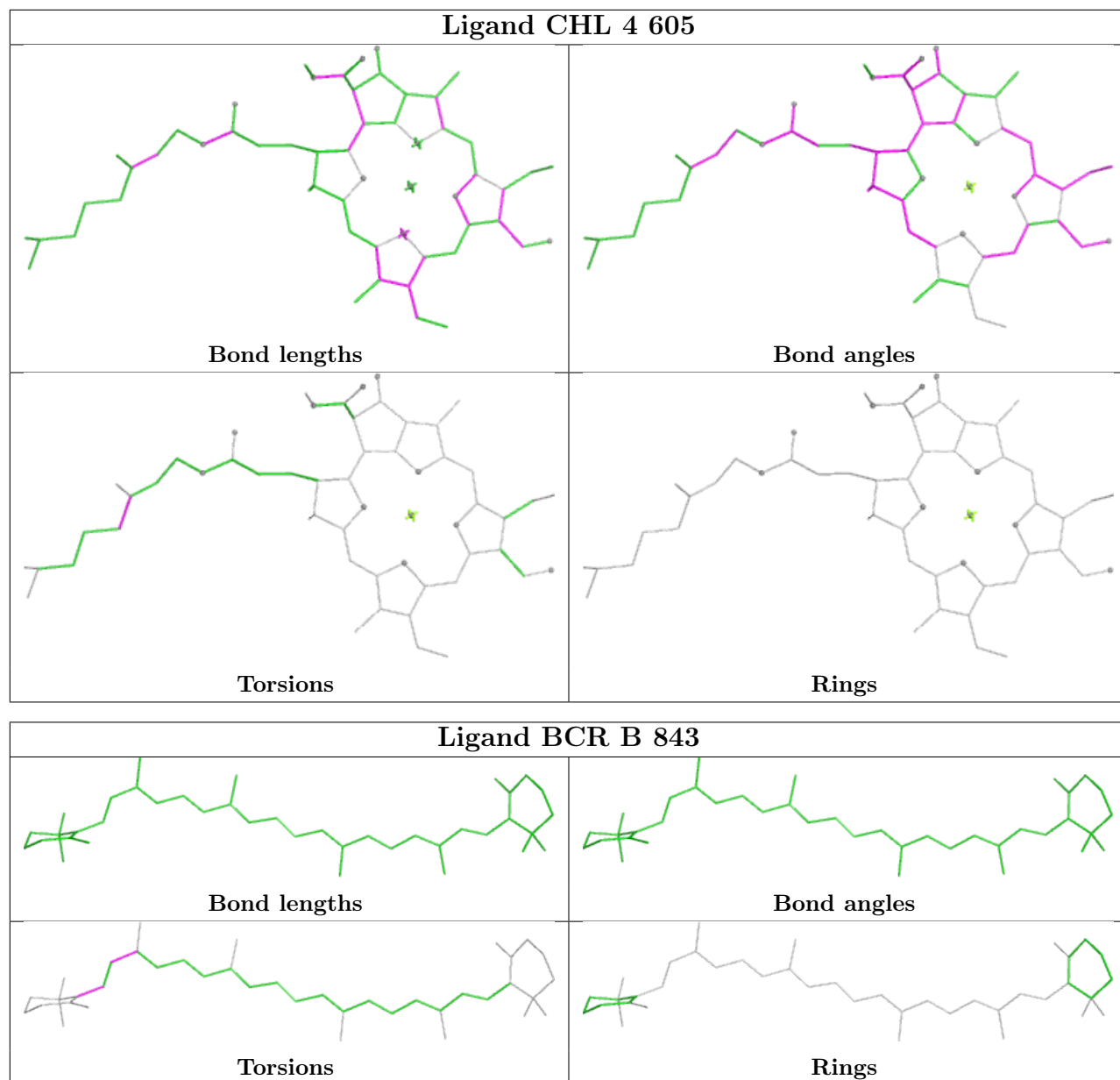
Ligand BCR B 845

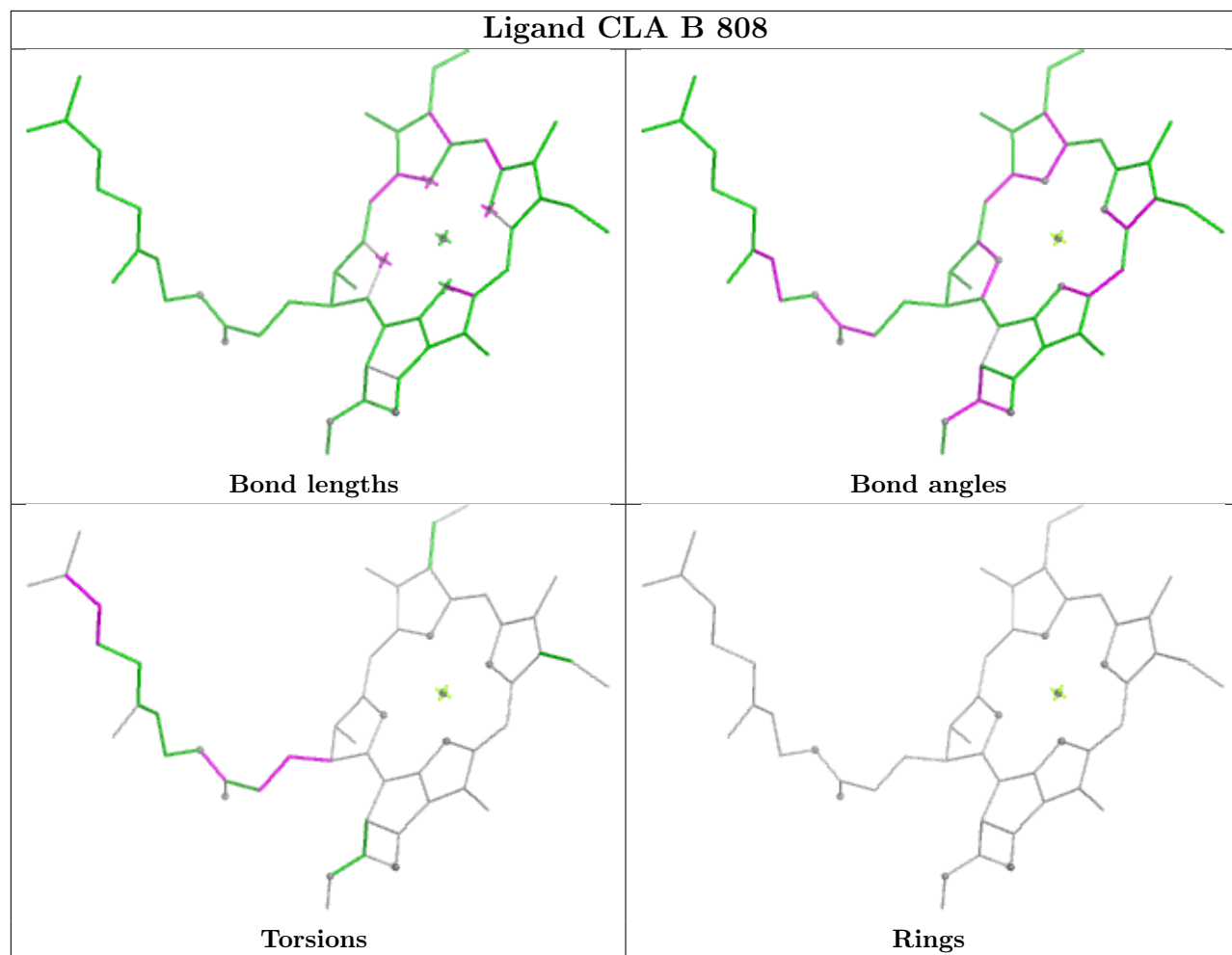




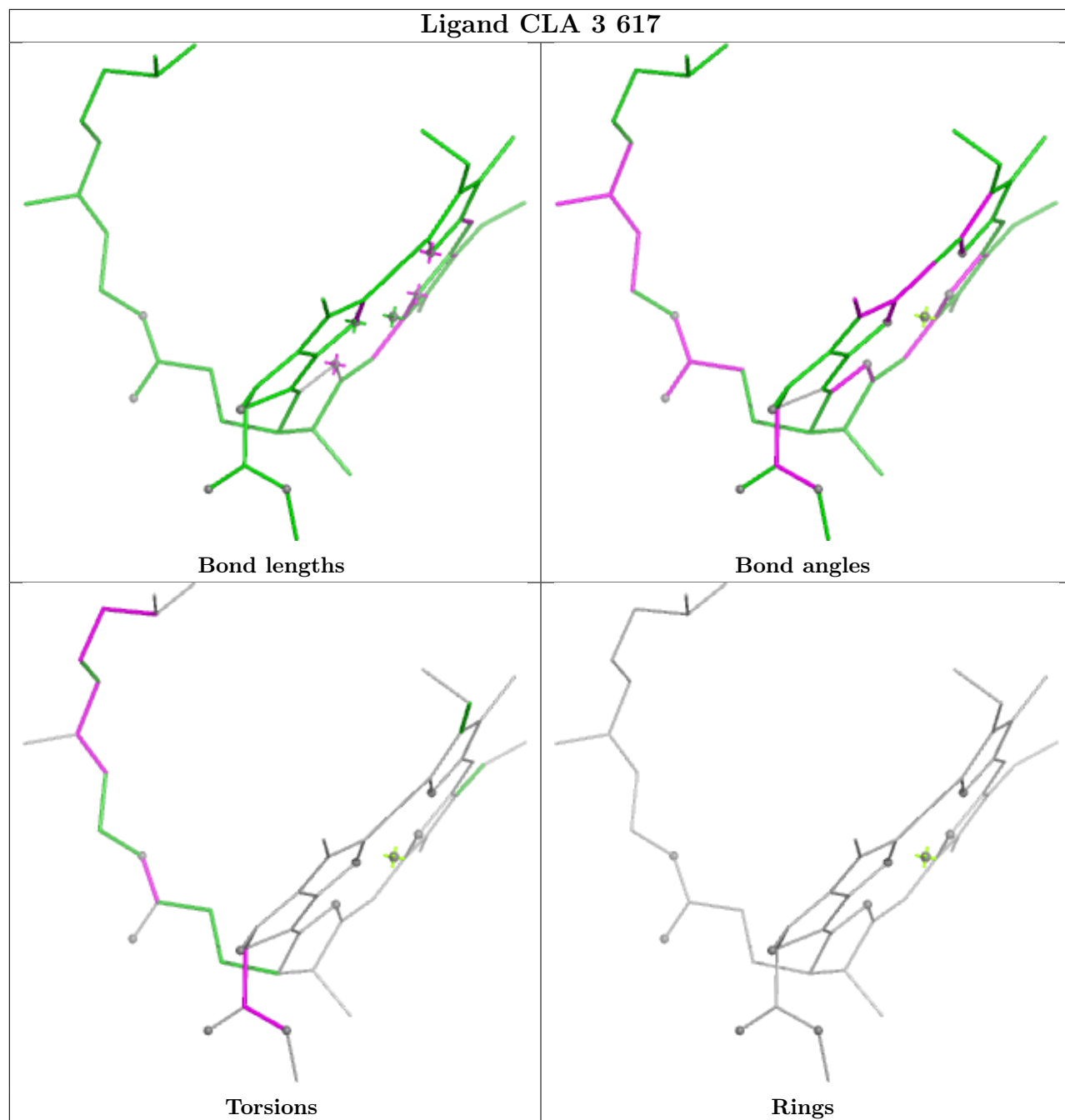




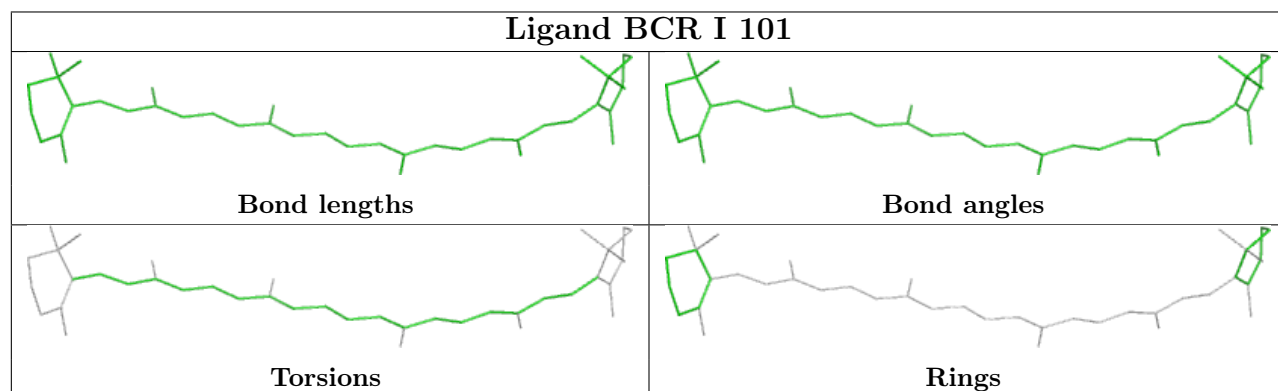




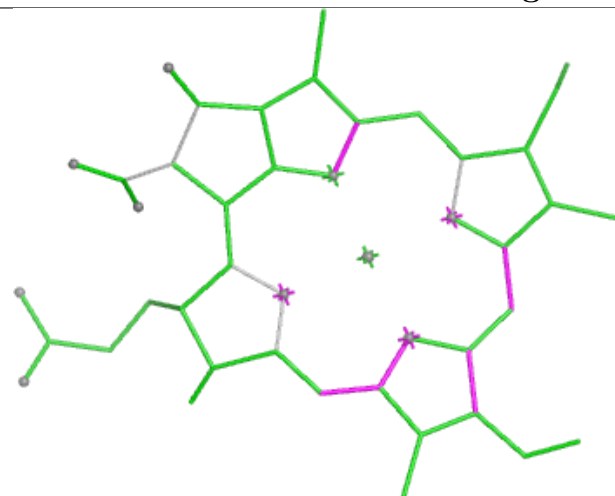
Ligand CLA 3 617



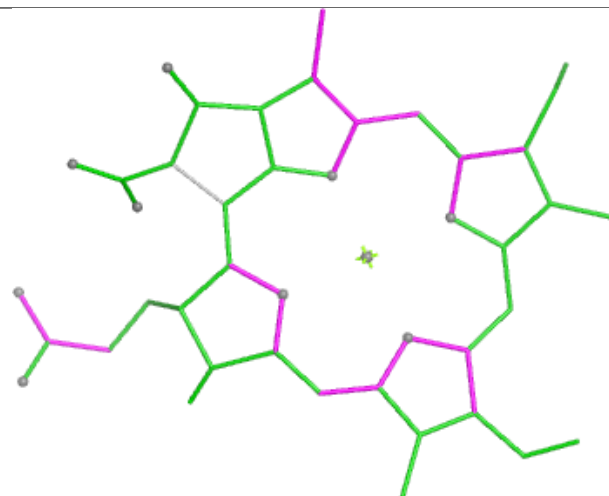
Ligand BCR I 101



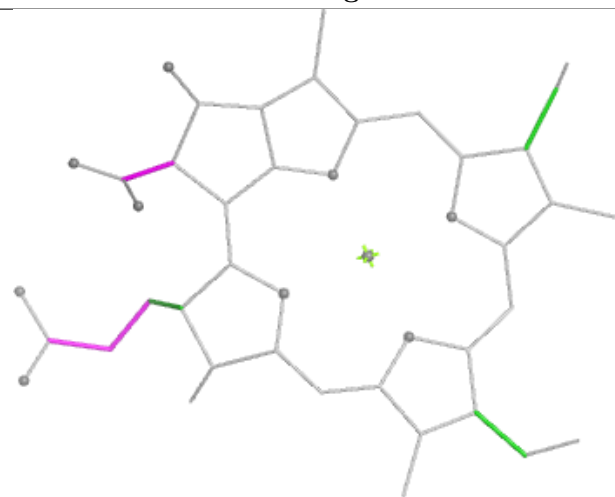
Ligand CLA 2 603



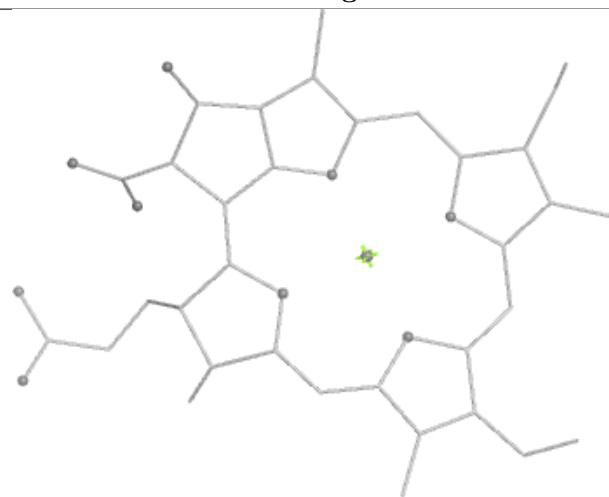
Bond lengths



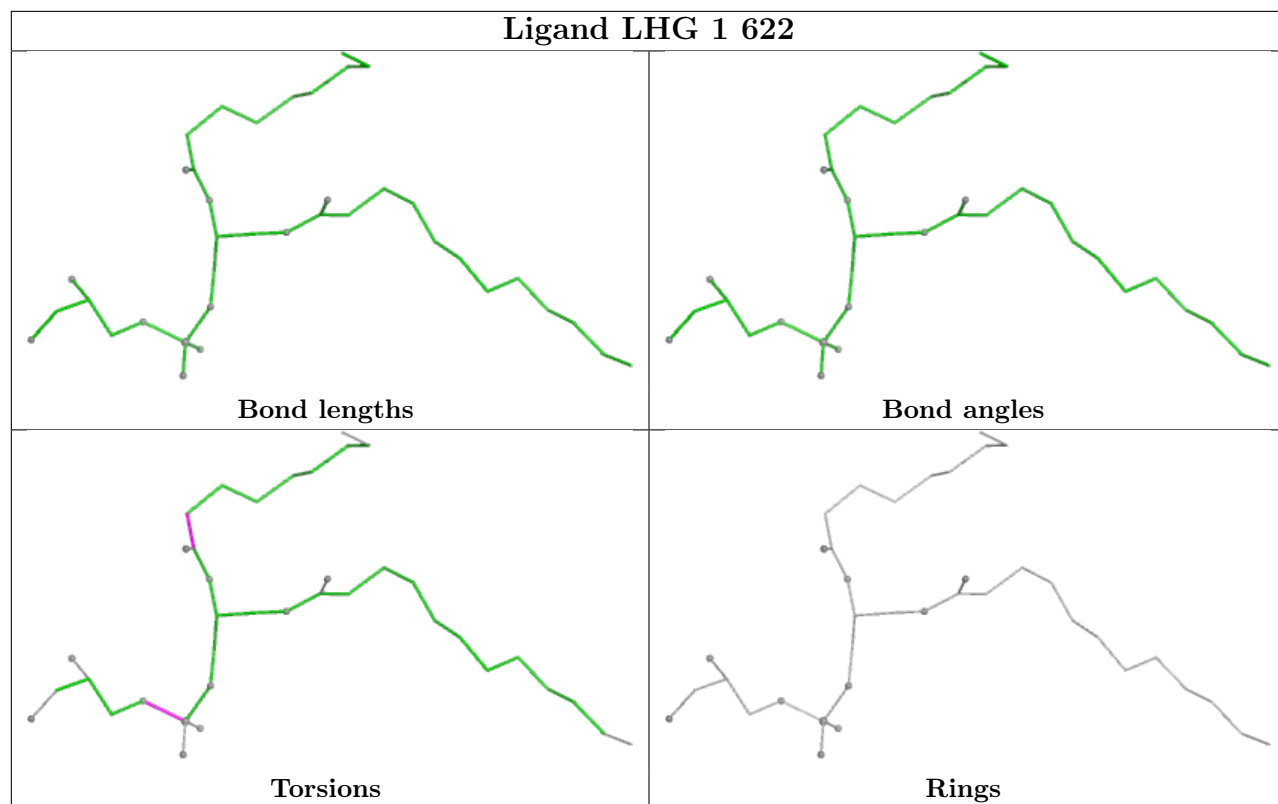
Bond angles



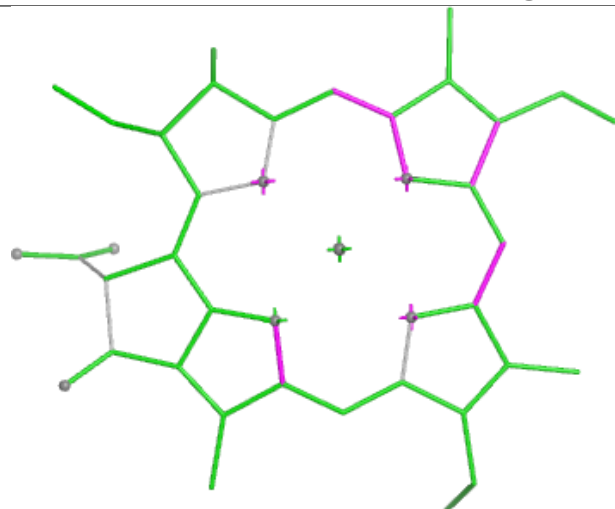
Torsions



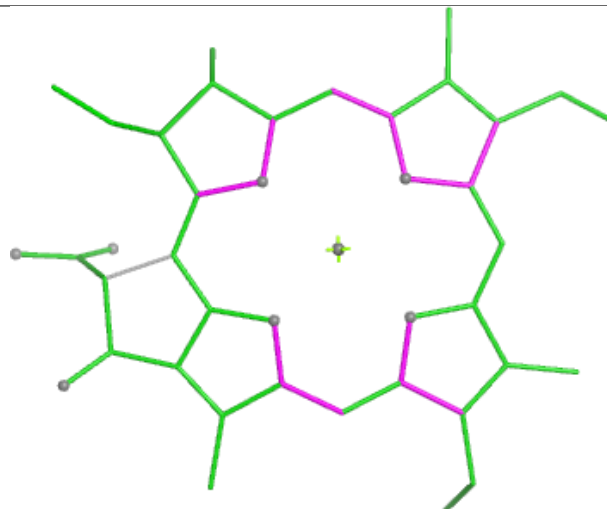
Rings



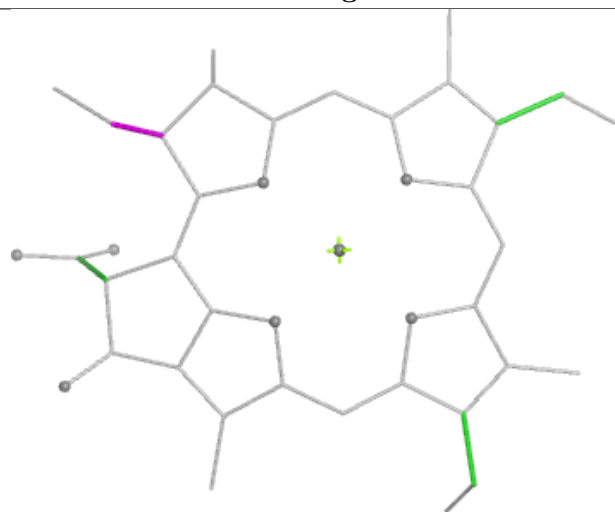
Ligand CLA 4 611



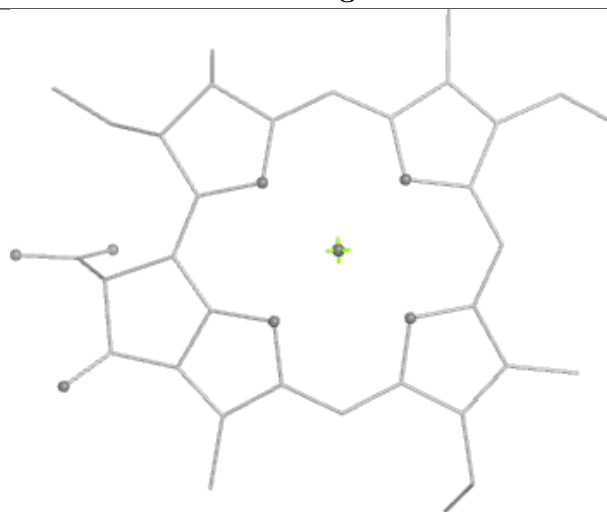
Bond lengths



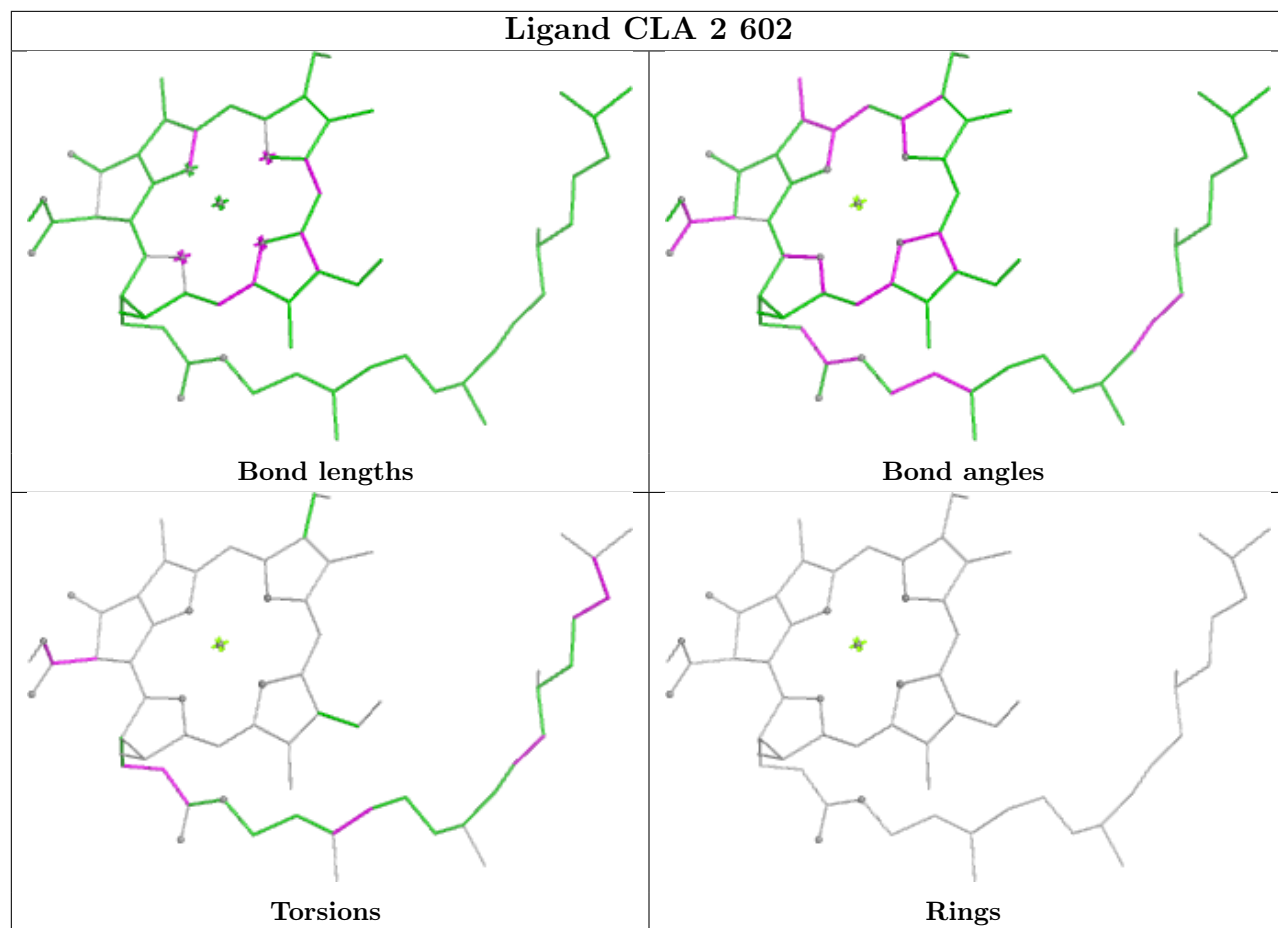
Bond angles

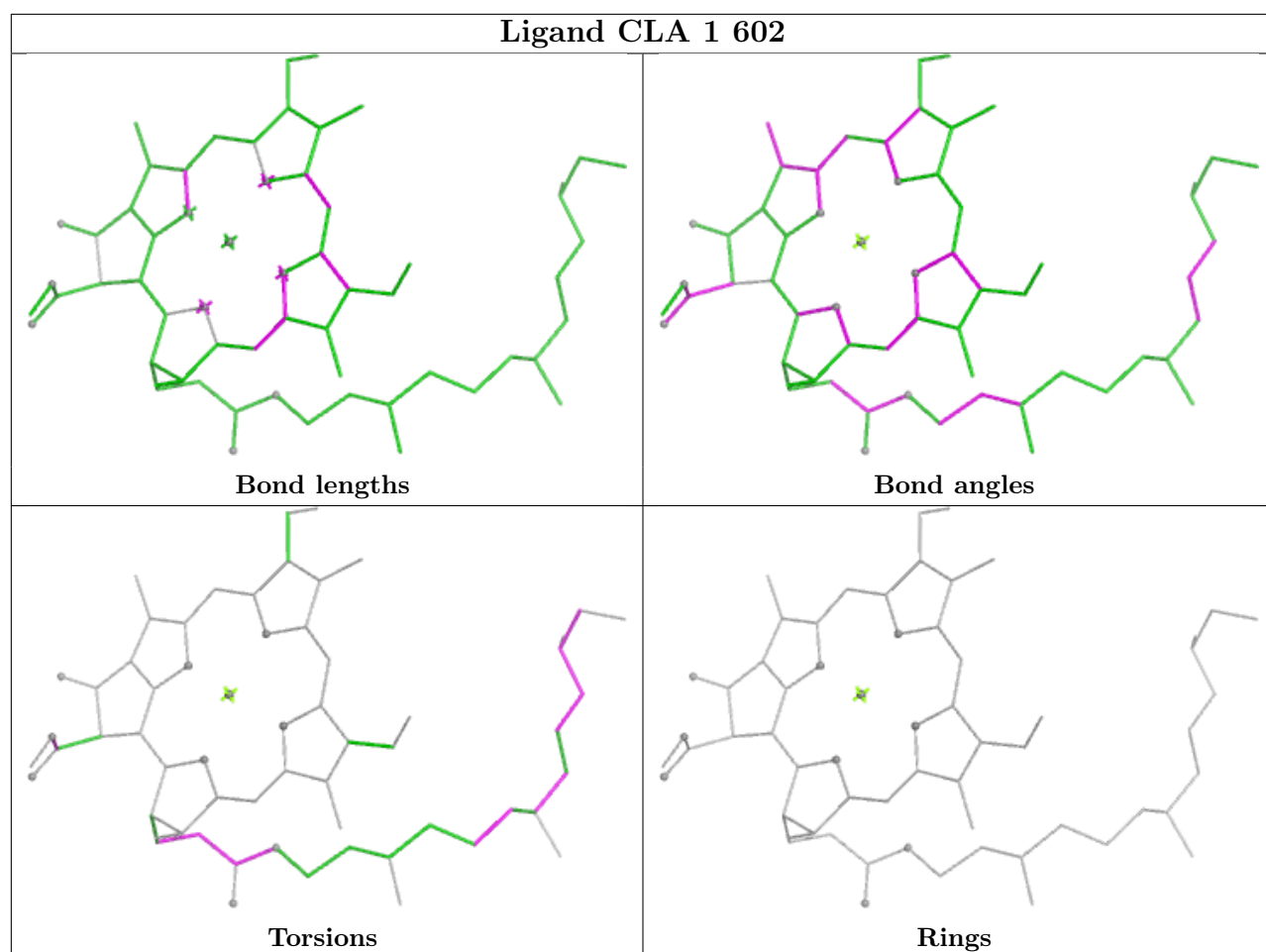


Torsions

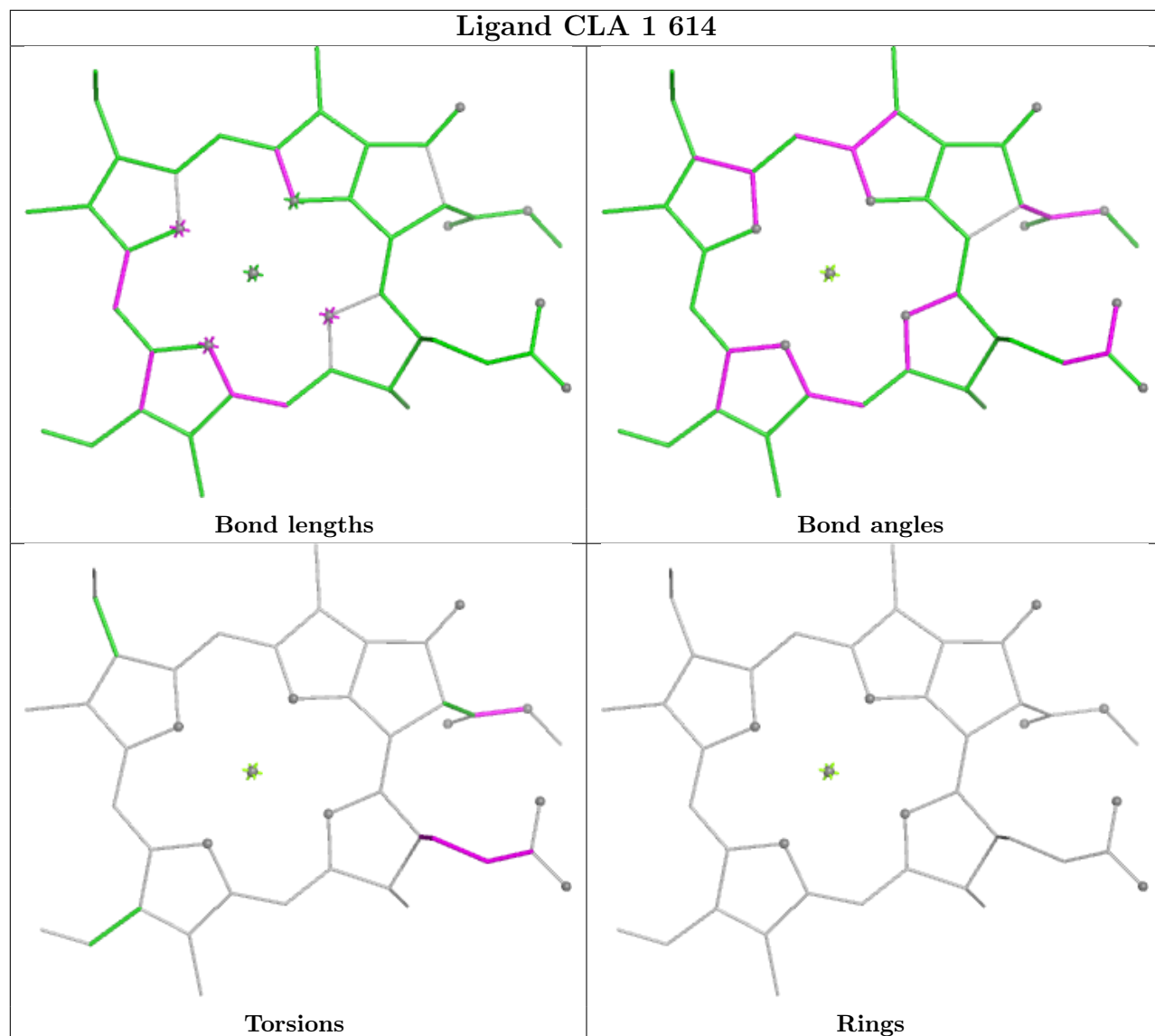


Rings

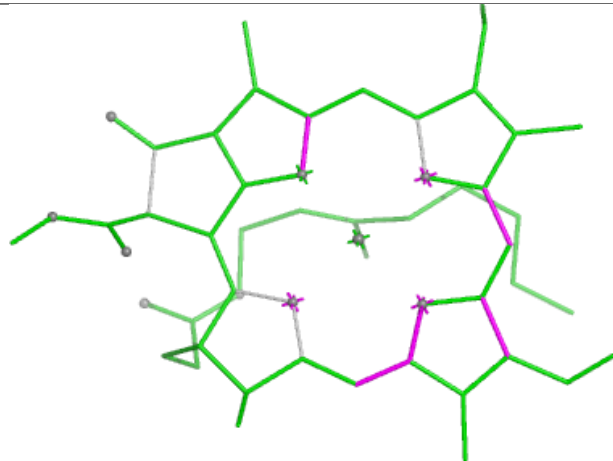




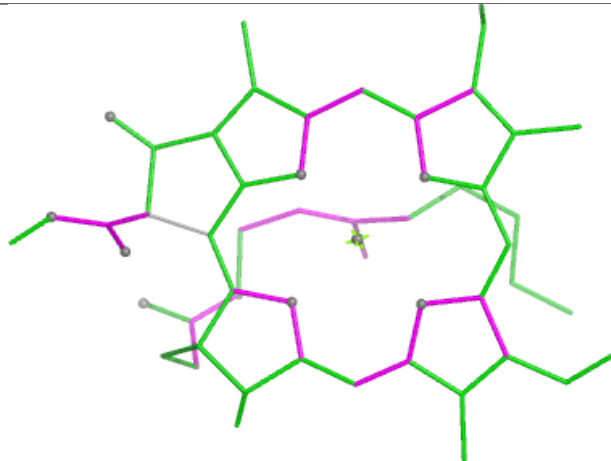
Ligand CLA 1 614



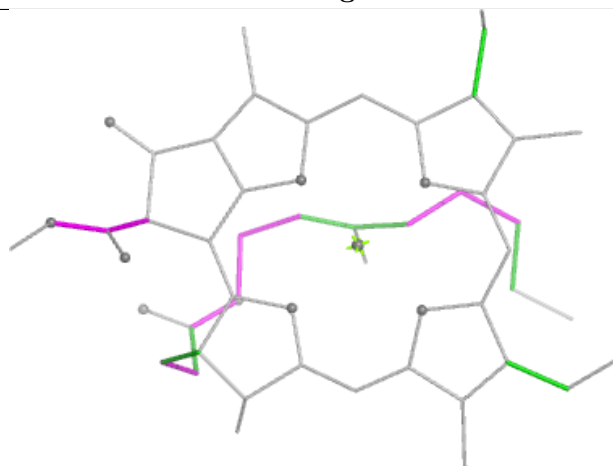
Ligand CLA A 812



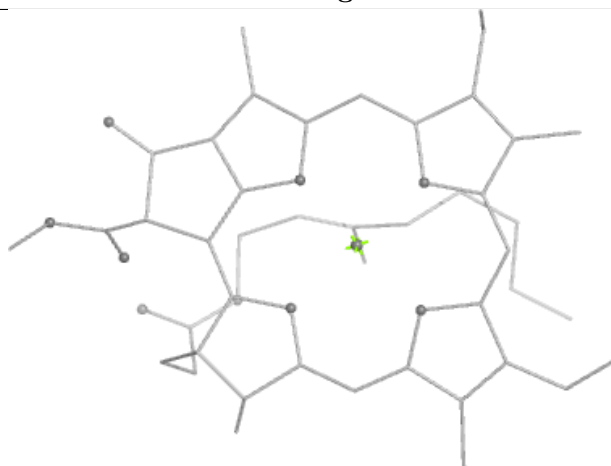
Bond lengths



Bond angles

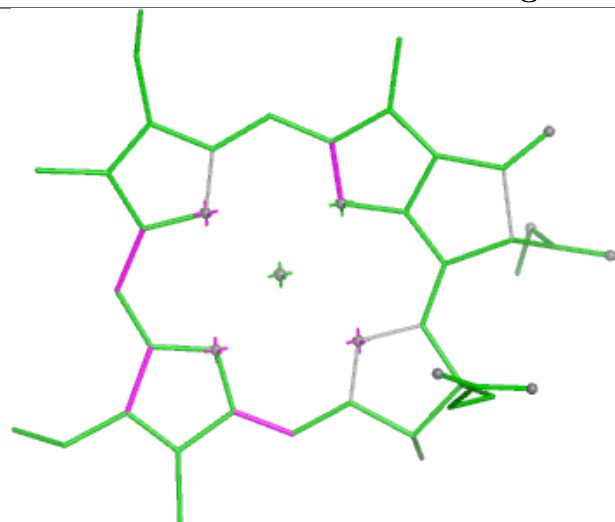


Torsions

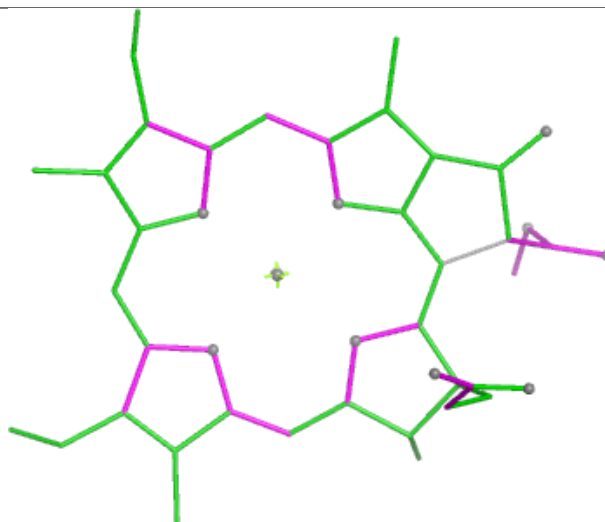


Rings

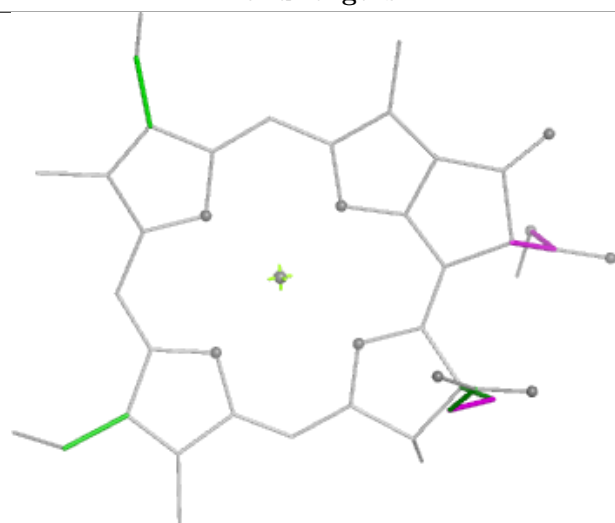
Ligand CLA 4 604



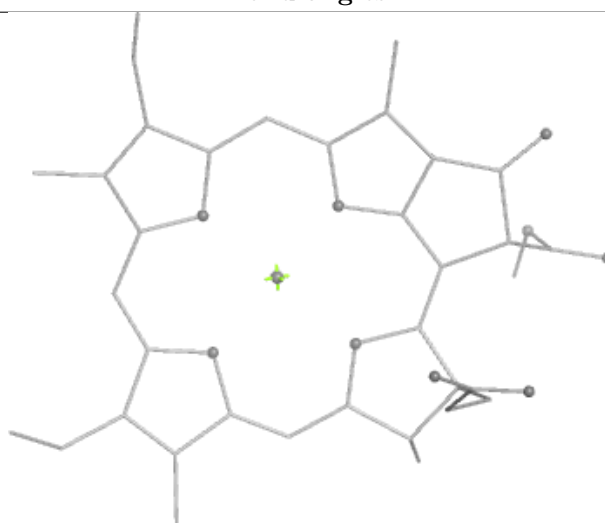
Bond lengths



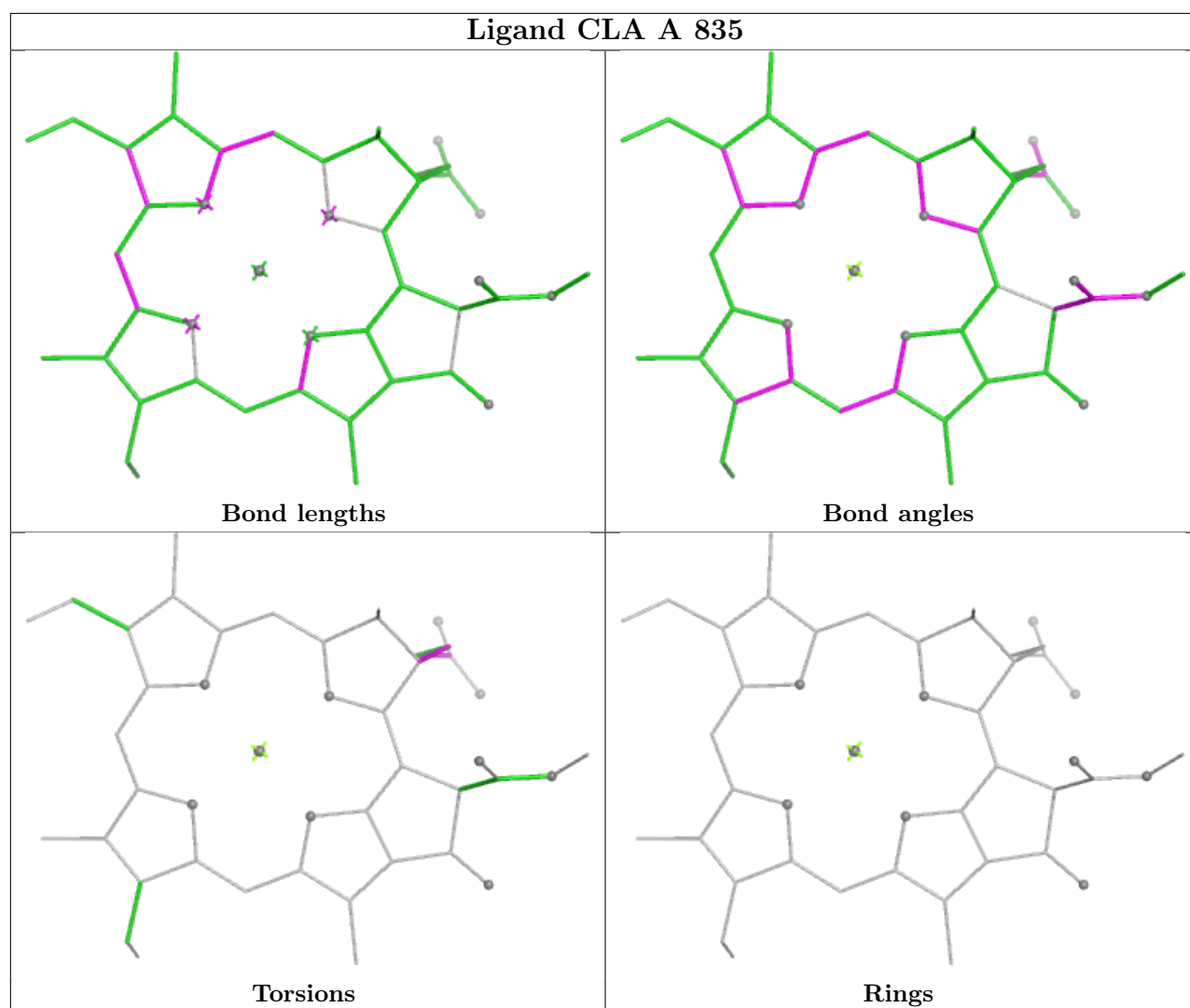
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

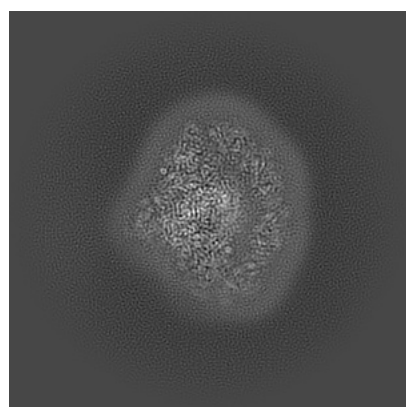
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54455. These allow visual inspection of the internal detail of the map and identification of artifacts.

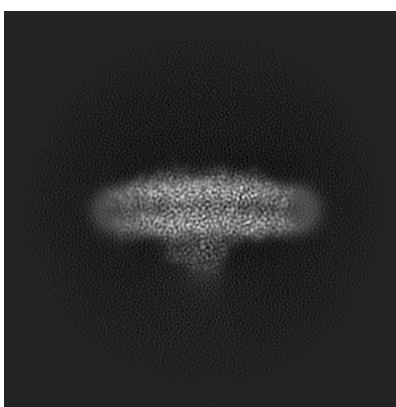
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

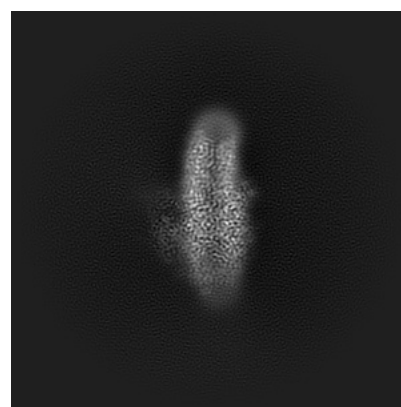
6.1.1 Primary map



X



Y

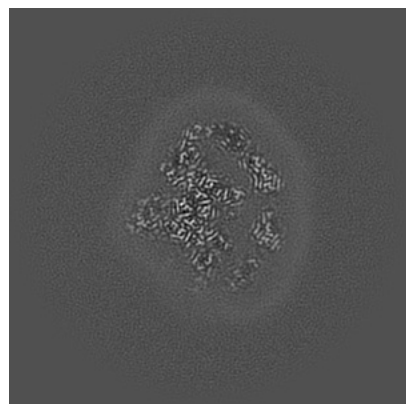


Z

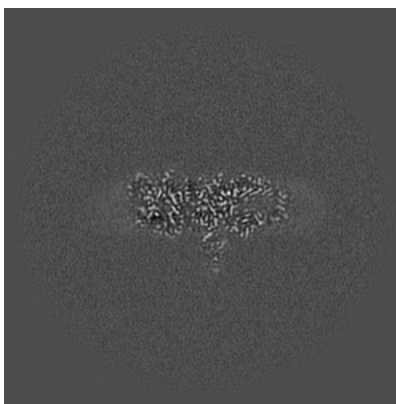
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

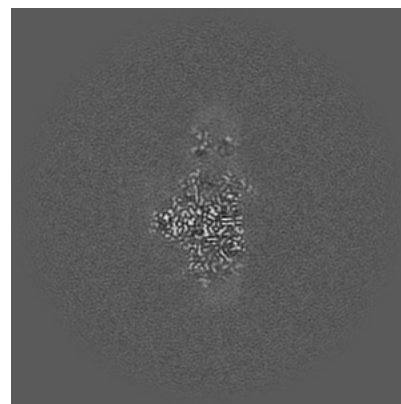
6.2.1 Primary map



X Index: 200



Y Index: 200

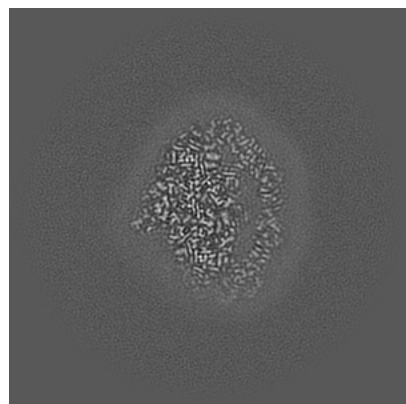


Z Index: 200

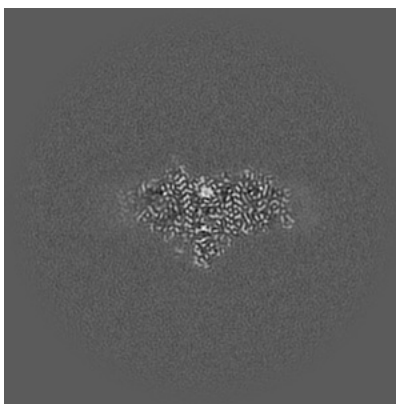
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

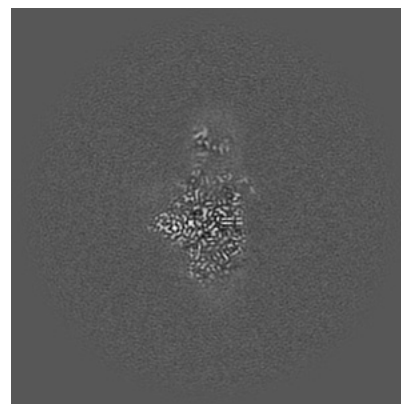
6.3.1 Primary map



X Index: 215



Y Index: 184

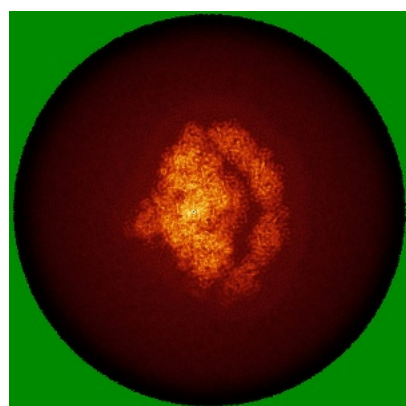


Z Index: 198

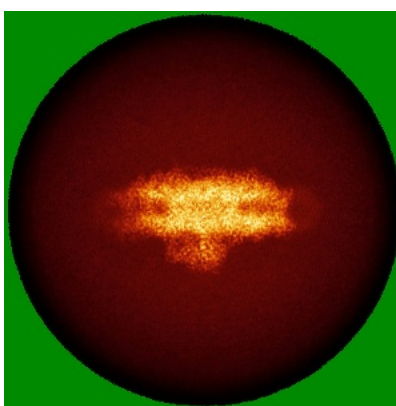
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

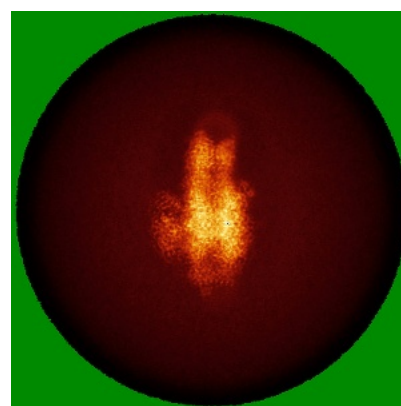
6.4.1 Primary map



X



Y

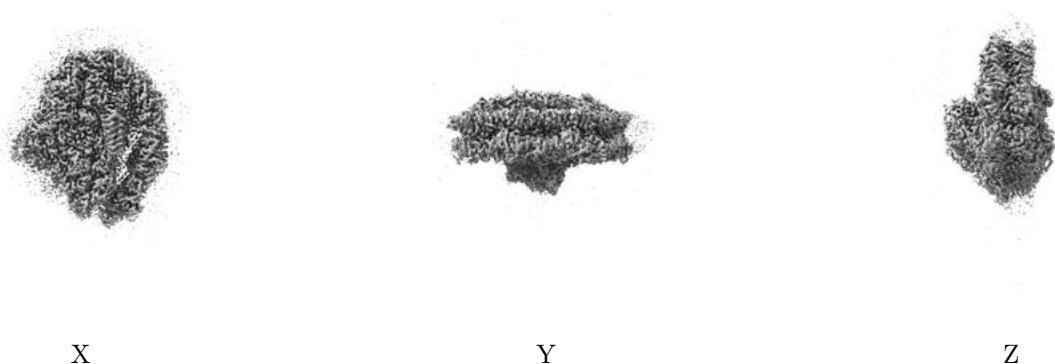


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

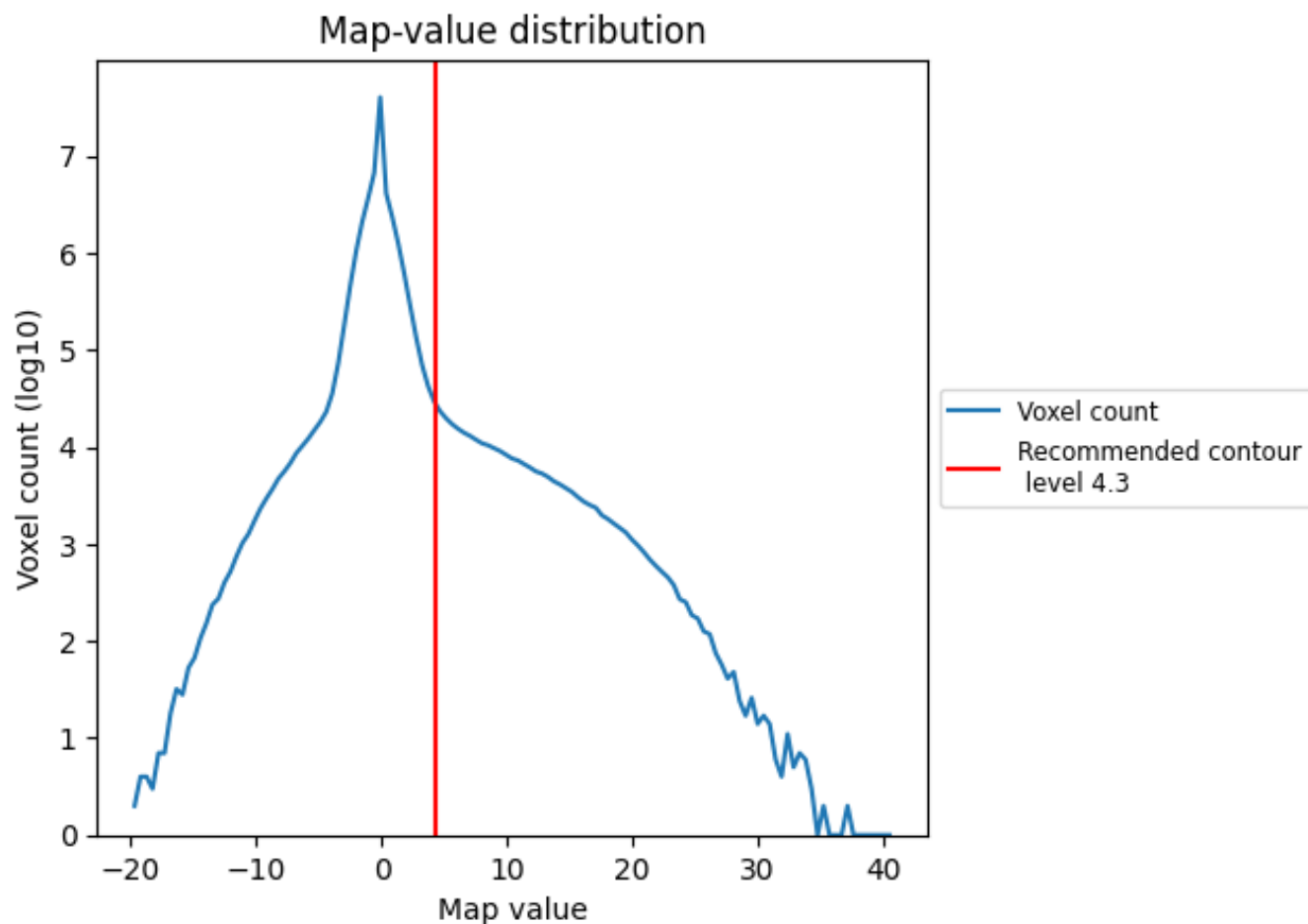
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

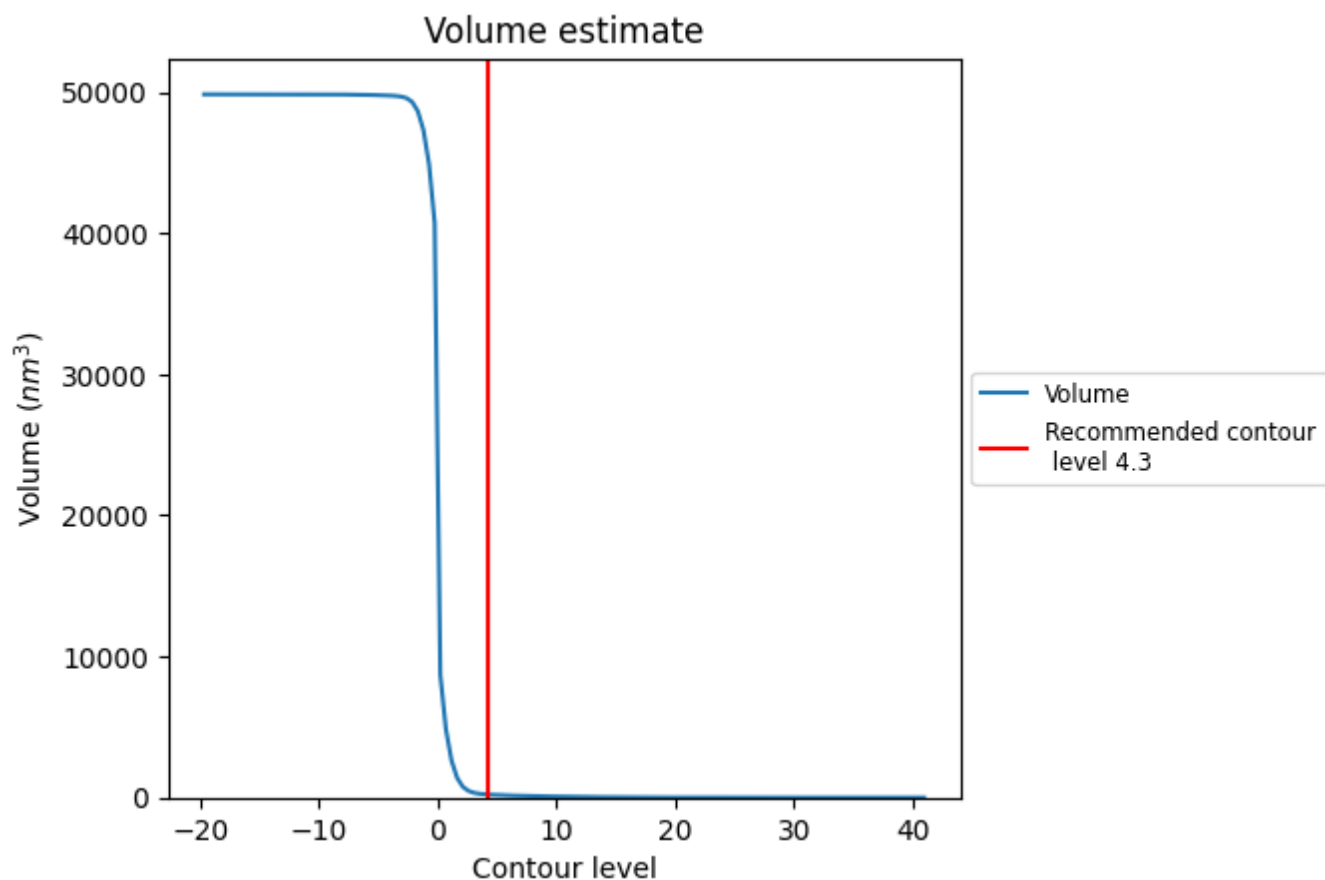
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

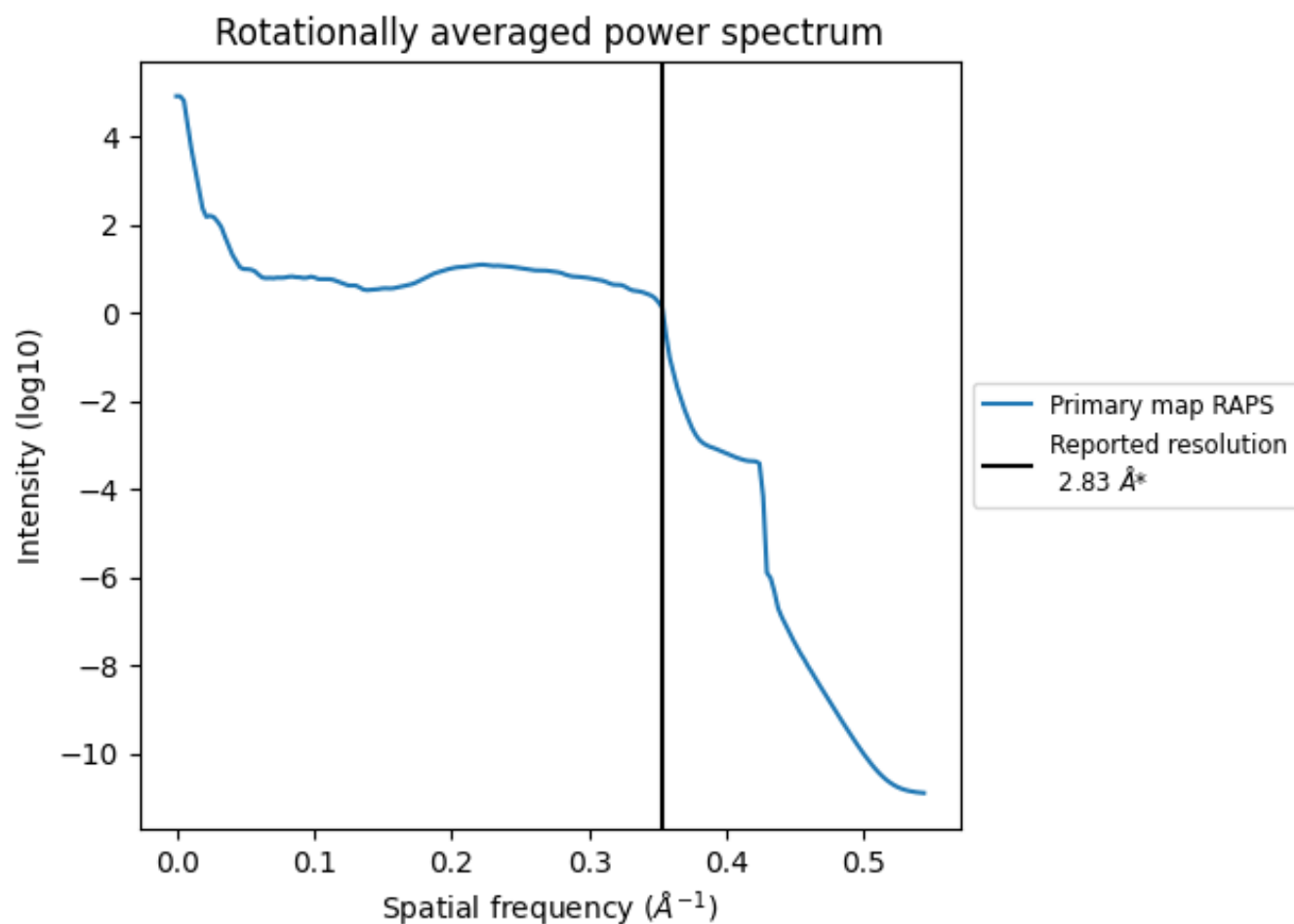
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 212 nm^3 ; this corresponds to an approximate mass of 192 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.353 Å⁻¹

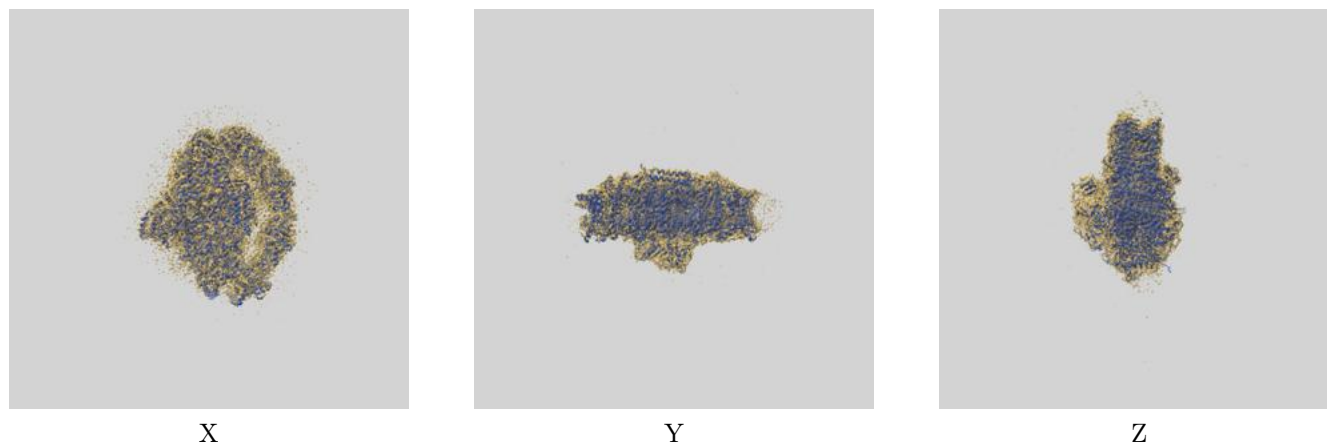
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

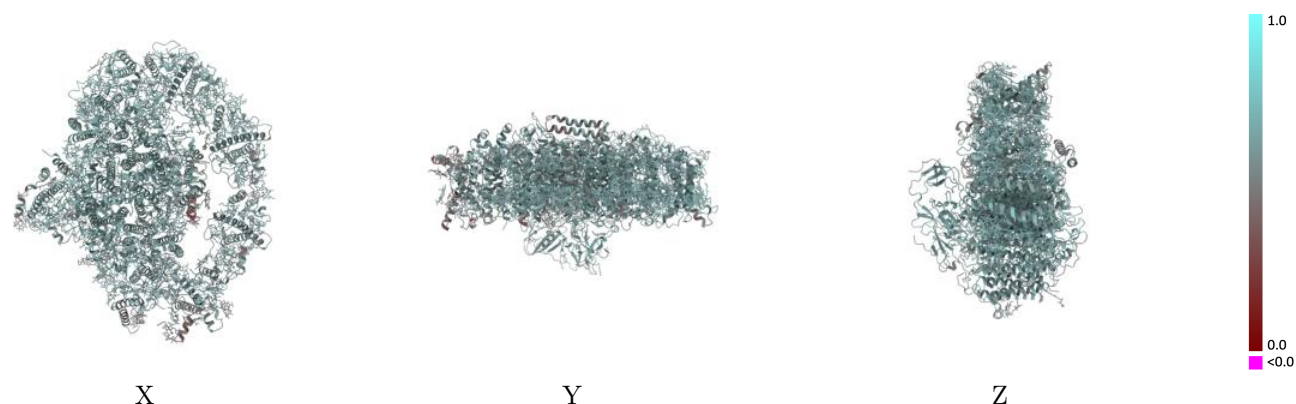
This section contains information regarding the fit between EMDB map EMD-54455 and PDB model 9S1L. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)



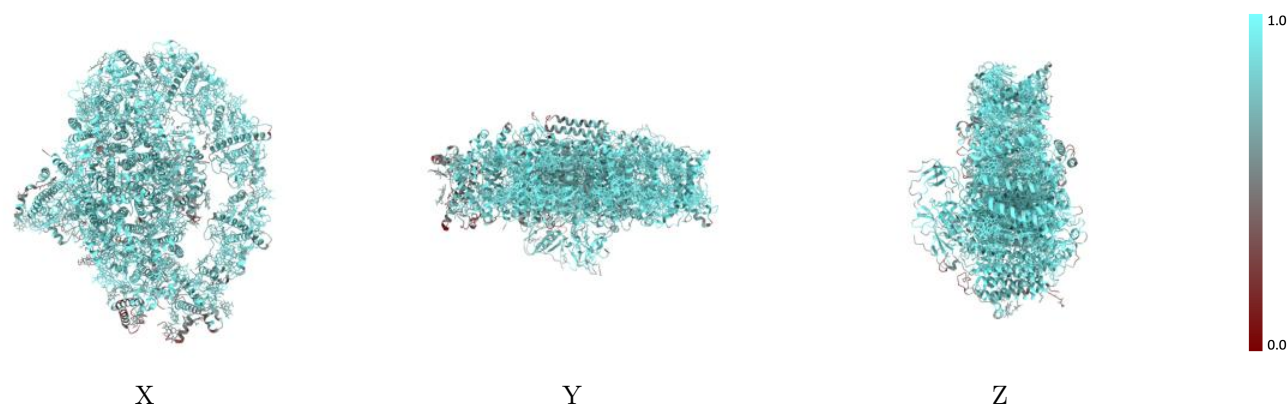
The images above show the 3D surface view of the map at the recommended contour level 4.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



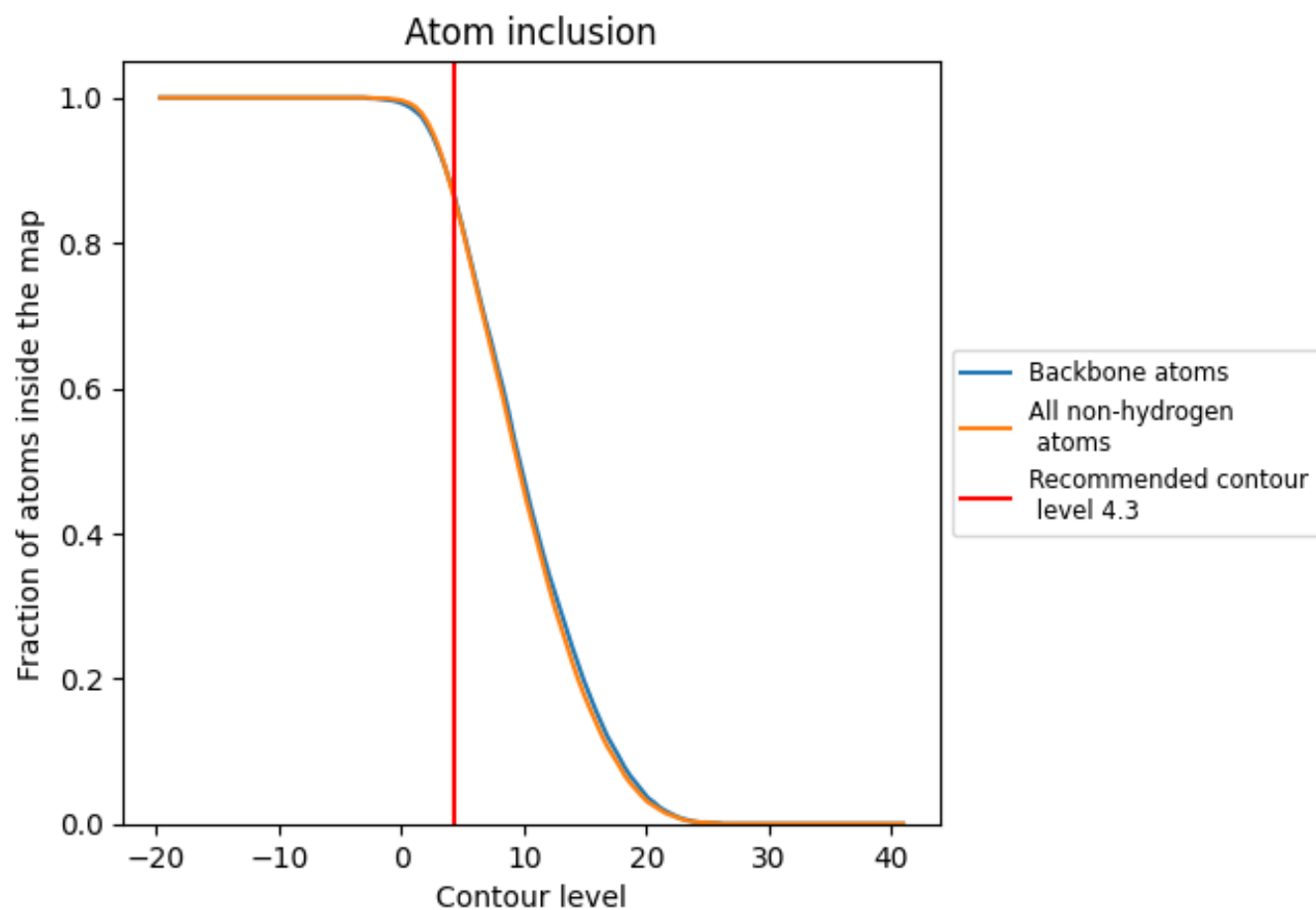
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8630	0.5940
1	0.8810	0.5940
2	0.8480	0.5650
3	0.6900	0.5240
4	0.8740	0.5890
A	0.9050	0.6120
B	0.9380	0.6240
C	0.9280	0.6080
D	0.8550	0.5960
E	0.8450	0.5930
F	0.7980	0.5730
G	0.8770	0.5950
H	0.6370	0.5330
I	0.8880	0.5990
J	0.7290	0.5240
K	0.4710	0.4880
L	0.7980	0.5810

